

azepane-2-thione

Other names:	.epsilon.-caprothiolactam 1-aza-2-cycloheptanethione hexahydro-2H-azepine-2-thione
Inchi:	InChI=1S/C6H11NS/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)
InchiKey:	APLHDUWNMGJBFD-UHFFFAOYSA-N
Formula:	C6H11NS
SMILES:	S=C1CCCCCN1
Mol. weight [g/mol]:	129.23

Physical Properties

Property code	Value	Unit	Source
gf	198.26	kJ/mol	Joback Method
hf	54.24	kJ/mol	Joback Method
hfus	15.58	kJ/mol	Joback Method
hvap	44.10	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.477		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4809.16	kPa	Joback Method
tb	486.36	K	Joback Method
tc	734.55	K	Joback Method
tf	334.18	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.11	J/mol×K	486.36	Joback Method
cpg	224.58	J/mol×K	527.72	Joback Method
cpg	238.09	J/mol×K	569.09	Joback Method
cpg	250.69	J/mol×K	610.45	Joback Method
cpg	262.42	J/mol×K	651.82	Joback Method
cpg	273.32	J/mol×K	693.18	Joback Method
cpg	283.42	J/mol×K	734.55	Joback Method

hvapt	98.20	kJ/mol	386.11	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	1.49e-04	kPa	322.08	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	1.21e-04	kPa	320.16	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	1.47e-04	kPa	322.08	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	1.90e-04	kPa	324.20	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	2.41e-04	kPa	326.15	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	2.87e-04	kPa	328.08	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	3.70e-04	kPa	330.18	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	4.68e-04	kPa	332.12	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	5.50e-04	kPa	334.07	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	7.08e-04	kPa	336.18	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	8.97e-04	kPa	338.15	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam

psub	1.05e-03	kPa	340.08	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	9.18e-05	kPa	318.18	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	1.20e-04	kPa	320.16	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	9.46e-05	kPa	318.18	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	1.81e-04	kPa	324.20	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	2.35e-04	kPa	326.15	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	2.88e-04	kPa	328.08	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	3.57e-04	kPa	330.18	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	4.54e-04	kPa	332.12	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	5.57e-04	kPa	334.07	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	6.86e-04	kPa	336.18	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	8.66e-04	kPa	338.15	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam

psub	1.06e-03	kPa	340.08	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	9.11e-05	kPa	318.18	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	1.17e-04	kPa	320.16	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	1.48e-04	kPa	322.08	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	1.82e-04	kPa	324.20	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	2.30e-04	kPa	326.15	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	2.89e-04	kPa	328.08	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	3.53e-04	kPa	330.18	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	4.42e-04	kPa	332.12	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	5.56e-04	kPa	334.07	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	6.76e-04	kPa	336.18	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
psub	8.43e-04	kPa	338.15	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam

psub

1.06e-03

kPa

340.08

Thermodynamic
properties of
epsilon-caprolactam
and
epsilon-caprothiolactam

Sources

McGowan Method:<http://link.springer.com/article/10.1007/BF02311772>**Crippen Method:**<http://pubs.acs.org/doi/abs/10.1021/ci990307l>**Crippen Method:**https://www.chemeo.com/doc/models/crippen_log10ws**Thermodynamic properties of
epsilon-caprolactam and
epsilon-caprothiolactam:**<https://www.doi.org/10.1016/j.jct.2019.01.014>**Joback Method:**https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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