

2-methyl-1,4-dithiepane

Other names:	1,4-Dithiacycloheptane, 3-methyl
Inchi:	InChI=1S/C6H12S2/c1-6-5-7-3-2-4-8-6/h6H,2-5H2,1H3
InchiKey:	RSKLGGRVBKLLIF-UHFFFAOYSA-N
Formula:	C6H12S2
SMILES:	CC1CSCCCS1
Mol. weight [g/mol]:	148.29

Physical Properties

Property code	Value	Unit	Source
gf	91.71	kJ/mol	Joback Method
hf	-28.49	kJ/mol	Joback Method
hfus	8.34	kJ/mol	Joback Method
hvap	41.18	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.245		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	1161.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1160.00		NIST Webbook
ripol	1635.00		NIST Webbook
tb	456.16	K	Joback Method
tc	705.33	K	Joback Method
tf	328.14	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.08	J/molxK	456.16	Joback Method
cpg	240.57	J/molxK	497.69	Joback Method
cpg	256.06	J/molxK	539.22	Joback Method
cpg	270.59	J/molxK	580.75	Joback Method

cpg	284.16	J/mol×K	622.27	Joback Method
cpg	296.82	J/mol×K	663.80	Joback Method
cpg	308.58	J/mol×K	705.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R82366&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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