

2,3,4,6-tetrathiaheptane

Inchi:	InChI=1S/C3H8S4/c1-4-3-6-7-5-2/h3H2,1-2H3
InchiKey:	PNXBHYQFLOGVCJ-UHFFFAOYSA-N
Formula:	C3H8S4
SMILES:	CSCSSSC
Mol. weight [g/mol]:	172.36

Physical Properties

Property code	Value	Unit	Source
gf	106.86	kJ/mol	Joback Method
hf	62.23	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	49.54	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.966		Crippen Method
mcvol	118.530	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1352.00		NIST Webbook
tb	543.16	K	Joback Method
tc	815.04	K	Joback Method
tf	261.17	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.81	J/molxK	543.16	Joback Method
cpg	225.24	J/molxK	588.47	Joback Method
cpg	234.13	J/molxK	633.79	Joback Method
cpg	242.44	J/molxK	679.10	Joback Method
cpg	250.12	J/molxK	724.42	Joback Method
cpg	257.12	J/molxK	769.73	Joback Method
cpg	263.40	J/molxK	815.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R226352&Units=SI
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

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
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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