2,2-dimethyl-3,5-dithiaheptane

Inchi: InChI=1S/C7H16S2/c1-5-8-6-9-7(2,3)4/h5-6H2,1-4H3
InchiKey: LHPISXNQYOGYGN-UHFFFAOYSA-N
Formula: C7H16S2
SMILES: CCSCSC(C)(C)C
Mol. weight [g/mol]: 164.33

Physical Properties

Property code	Value	Unit	Source
gf	77.14	kJ/mol	Joback Method
hf	-112.82	kJ/mol	Joback Method
hfus	14.73	kJ/mol	Joback Method
hvap	43.51	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.229		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	1154.00		NIST Webbook
rinpol	1154.00		NIST Webbook
tb	493.89	K	Joback Method
tc	717.04	K	Joback Method
tf	239.87	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.52	J/mol×K	493.89	Joback Method
cpg	314.16	J/mol×K	531.08	Joback Method
cpg	327.96	J/mol×K	568.27	Joback Method
cpg	340.94	J/mol×K	605.47	Joback Method
cpg	353.13	J/mol×K	642.66	Joback Method
cpg	364.54	J/mol×K	679.85	Joback Method
cpg	375.22	J/mol×K	717.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155349&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume