3-methyl-2,4-dithia-6-heptene

Inchi: InChI=1S/C6H12S2/c1-4-5-8-6(2)7-3/h4,6H,1,5H2,2-3H3
InchiKey: HZLVRNMVTBTNMN-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: C=CCSC(C)SC
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	151.28	kJ/mol	Joback Method
hf	36.72	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	41.53	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.615		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
tb	470.48	K	Joback Method
tc	692.73	K	Joback Method
tf	209.42	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.35	J/mol×K	470.48	Joback Method
cpg	249.25	J/mol×K	507.52	Joback Method
cpg	260.57	J/mol×K	544.56	Joback Method
cpg	271.30	J/mol×K	581.61	Joback Method
cpg	281.46	J/mol×K	618.65	Joback Method
cpg	291.04	J/mol×K	655.69	Joback Method
cpg	300.07	J/mol×K	692.73	Joback Method

Sources

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=R156664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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