2,4,4-trimethyl-3,5-dithiahexane

Inchi: InChI=1S/C7H16S2/c1-6(2)9-7(3,4)8-5/h6H,1-5H3
InchiKey: XKBRTPMCDMZXEH-UHFFFAOYSA-N
Formula: C7H16S2
SMILES: CSC(C)(C)SC(C)C
Mol. weight [g/mol]: 164.33

Physical Properties

Property code	Value	Unit	Source
gf	74.70	kJ/mol	Joback Method
hf	-118.10	kJ/mol	Joback Method
hfus	11.21	kJ/mol	Joback Method
hvap	43.13	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.227		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1089.00		NIST Webbook
rinpol	1089.00		NIST Webbook
tb	493.45	K	Joback Method
tc	721.94	K	Joback Method
tf	224.87	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.74	J/mol×K	493.45	Joback Method
cpg	314.82	J/mol×K	531.53	Joback Method
cpg	329.00	J/mol×K	569.61	Joback Method
cpg	342.32	J/mol×K	607.69	Joback Method
cpg	354.78	J/mol×K	645.77	Joback Method
cpg	366.44	J/mol×K	683.86	Joback Method
cpg	377.31	J/mol×K	721.94	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=R155567&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