2,4,5-Trithiahexane, 3-(2-methylpropyl)

Inchi: InChI=1S/C7H16S3/c1-6(2)5-7(8-3)10-9-4/h6-7H,5H2,1-4H3
InchiKey: LJIWXNLJDUSJOD-UHFFFAOYSA-N
Formula: C7H16S3
SMILES: CSSC(CC(C)C)SC
Mol. weight [g/mol]: 196.40
CAS: 69078-82-6

Physical Properties

Property code	Value	Unit	Source
gf	102.54	kJ/mol	Joback Method
hf	-72.76	kJ/mol	Joback Method
hfus	19.23	kJ/mol	Joback Method
hvap	50.85	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.733		Crippen Method
mcvol	158.540	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	1370.00		NIST Webbook
tb	565.02	K	Joback Method
tc	804.77	K	Joback Method
tf	241.85	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.43	J/mol×K	565.02	Joback Method
cpg	362.12	J/mol×K	604.98	Joback Method
cpg	375.97	J/mol×K	644.94	Joback Method
cpg	388.98	J/mol×K	684.90	Joback Method
cpg	401.13	J/mol×K	724.85	Joback Method
cpg	412.42	J/mol×K	764.81	Joback Method
cpg	422.86	J/mol×K	804.77	Joback Method

Sources

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=C69078826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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