Hexane, 2,3-bis-(methylthio), threo

Inchi: InChI=1S/C8H18S2/c1-5-6-8(10-4)7(2)9-3/h7-8H,5-6H2,1-4H3/t7-,8-/m0/s1
InchiKey: CWHNWBBWKOZADZ-YUMQZZPRSA-N
Formula: C8H18S2
SMILES: CCCC(SC)C(C)SC
Mol. weight [g/mol]: 178.36

Physical Properties

Property code	Value	Unit	Source
gf	77.84	kJ/mol	Joback Method
hf	-135.27	kJ/mol	Joback Method
hfus	17.69	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.270		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1287.00		NIST Webbook
rinpol	1287.00		NIST Webbook
tb	519.12	K	Joback Method
tc	734.48	K	Joback Method
tf	218.72	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.26	J/mol×K	519.12	Joback Method
cpg	356.56	J/mol×K	555.01	Joback Method
cpg	371.10	J/mol×K	590.91	Joback Method
cpg	384.91	J/mol×K	626.80	Joback Method
cpg	397.97	J/mol×K	662.70	Joback Method
cpg	410.31	J/mol×K	698.59	Joback Method
cpg	421.93	J/mol×K	734.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121792&Units=SI

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