Heneicosane, 1,2-bis(methylthio)

Inchi: InChI=1S/C23H48S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23(25-3)22-2
InchiKey: OMUJQNFTNURUOB-UHFFFAOYSA-N
Formula: C23H48S2
SMILES: CCCCCCCCCCCCCCCCCCCC(CSC)SC
Mol. weight [g/mol]: 388.76

Physical Properties

Property code	Value	Unit	Source
gf	206.58	kJ/mol	Joback Method
hf	-439.59	kJ/mol	Joback Method
hfus	60.06	kJ/mol	Joback Method
hvap	80.04	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	9.123		Crippen Method
mcvol	367.630	ml/mol	McGowan Method
pc	873.25	kPa	Joback Method
rinpol	2907.00		NIST Webbook
rinpol	2907.00		NIST Webbook
tb	862.76	K	Joback Method
tc	1058.43	K	Joback Method
tf	402.77	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.02	J/mol×K	862.76	Joback Method
cpg	1200.92	J/mol×K	895.37	Joback Method
cpg	1220.55	J/mol×K	927.98	Joback Method
cpg	1238.96	J/mol×K	960.59	Joback Method
cpg	1256.19	J/mol×K	993.21	Joback Method
cpg	1272.29	J/mol×K	1025.82	Joback Method
cpg	1287.29	J/mol×K	1058.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R59090&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

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

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