Hexadecane, 2-methyl-1,2-bis(methylthio)

Inchi: InChI=1S/C19H40S2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-19(2,21-4)18-20-3/h5-18H2
InchiKey: BYSOCCVIZUKYQP-UHFFFAOYSA-N
Formula: C19H40S2
SMILES: CCCCCCCCCCCCCCC(C)(CSC)SC
Mol. weight [g/mol]: 332.65

Physical Properties

Property code	Value	Unit	Source
gf	178.18	kJ/mol	Joback Method
hf	-360.50	kJ/mol	Joback Method
hfus	45.81	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.562		Crippen Method
mcvol	311.270	ml/mol	McGowan Method
pc	1119.30	kPa	Joback Method
rinpol	2438.00		NIST Webbook
tb	768.45	K	Joback Method
tc	960.99	K	Joback Method
tf	375.11	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.25	J/mol×K	768.45	Joback Method
cpg	953.25	J/mol×K	800.54	Joback Method
cpg	972.13	J/mol×K	832.63	Joback Method
cpg	989.94	J/mol×K	864.72	Joback Method
cpg	1006.71	J/mol×K	896.81	Joback Method
cpg	1022.50	J/mol×K	928.90	Joback Method
cpg	1037.35	J/mol×K	960.99	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=R59143&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