Heptadecane, 1,2-bis(methylthio)

Inchi: InChI=1S/C19H40S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19(21-3)18-20-2/h19H,4-1
InchiKey: YPTGIARQRQFJIY-UHFFFAOYSA-N
Formula: C19H40S2
SMILES: CCCCCCCCCCCCCCCC(CSC)SC
Mol. weight [g/mol]: 332.65

Physical Properties

Property code	Value	Unit	Source
gf	172.90	kJ/mol	Joback Method
hf	-357.03	kJ/mol	Joback Method
hfus	49.70	kJ/mol	Joback Method
hvap	71.13	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.562		Crippen Method
mcvol	311.270	ml/mol	McGowan Method
pc	1111.11	kPa	Joback Method
rinpol	2477.00		NIST Webbook
rinpol	2477.00		NIST Webbook
tb	771.24	K	Joback Method
tc	960.17	K	Joback Method
tf	357.69	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.41	J/mol×K	771.24	Joback Method
cpg	952.29	J/mol×K	802.73	Joback Method
cpg	971.09	J/mol×K	834.22	Joback Method
cpg	988.82	J/mol×K	865.70	Joback Method
cpg	1005.53	J/mol×K	897.19	Joback Method
cpg	1021.24	J/mol×K	928.68	Joback Method
cpg	1035.98	J/mol×K	960.17	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=R59125&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