Octadecane, 1-(methylthio)-

Inchi: InChI=1S/C19H40S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-2/h3-19H2,1-2H
InchiKey: BNORDZYQJMGMRG-UHFFFAOYSA-N
Formula: C19H40S
SMILES: CCCCCCCCCCCCCCCCCCCSC
Mol. weight [g/mol]: 300.59
CAS: 40289-98-3

Physical Properties

Property code	Value	Unit	Source
gf	142.22	kJ/mol	Joback Method
hf	-393.62	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	64.70	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.611		Crippen Method
mcvol	294.920	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
tb	702.90	K	Joback Method
tc	876.28	K	Joback Method
tf	338.29	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.70	J/mol×K	702.90	Joback Method
cpg	878.97	J/mol×K	731.80	Joback Method
cpg	898.30	J/mol×K	760.69	Joback Method
cpg	916.73	J/mol×K	789.59	Joback Method
cpg	934.28	J/mol×K	818.49	Joback Method
cpg	950.98	J/mol×K	847.38	Joback Method
cpg	966.86	J/mol×K	876.28	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=C40289983&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume