1-Mercapto-2-heptadecanone

Inchi: InChI=1S/C17H34OS/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17(18)16-19/h19H,2-16H2,1
InchiKey: MNNWFOGLHGABKN-UHFFFAOYSA-N
Formula: C17H34OS
SMILES: CCCCCCCCCCCCCCCC(=O)CS
Mol. weight [g/mol]: 286.52
CAS: 76078-79-0

Physical Properties

Property code	Value	Unit	Source
gf	-7.27	kJ/mol	Joback Method
hf	-468.31	kJ/mol	Joback Method
hfus	45.43	kJ/mol	Joback Method
hvap	66.92	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	5.967		Crippen Method
mcvol	268.310	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
ripol	2397.00		NIST Webbook
ripol	2397.00		NIST Webbook
tb	705.09	K	Joback Method
tc	885.65	K	Joback Method
tf	367.74	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.61	J/mol×K	705.09	Joback Method
cpg	784.88	J/mol×K	735.18	Joback Method
cpg	802.26	J/mol×K	765.28	Joback Method
cpg	818.79	J/mol×K	795.37	Joback Method
cpg	834.48	J/mol×K	825.46	Joback Method
cpg	849.38	J/mol×K	855.56	Joback Method
cpg	863.51	J/mol×K	885.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76078790&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume