

Disulfide, dihexadecyl

Other names:	Hexadecyl disulfide dihexadecyl disulphide
Inchi:	InChI=1S/C32H66S2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-34-32-30-28-26-1
InchiKey:	GUBWMRCVCQFLOJ-UHFFFAOYSA-N
Formula:	C32H66S2
SMILES:	CCCCCCCCCCCCCCCCSSCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	515.00
CAS:	1561-75-7

Physical Properties

Property code	Value	Unit	Source
gf	284.80	kJ/mol	Joback Method
hf	-620.07	kJ/mol	Joback Method
hfus	86.90	kJ/mol	Joback Method
hvap	100.46	kJ/mol	Joback Method
log10ws	-13.98		Crippen Method
logp	13.330		Crippen Method
mcvol	494.440	ml/mol	McGowan Method
pc	552.07	kPa	Joback Method
tb	1069.12	K	Joback Method
tc	1339.46	K	Joback Method
tf	519.20	K	Joback Method
vc	1.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1768.78	J/mol×K	1069.12	Joback Method
cpg	1795.07	J/mol×K	1114.18	Joback Method
cpg	1818.99	J/mol×K	1159.23	Joback Method
cpg	1840.70	J/mol×K	1204.29	Joback Method
cpg	1860.38	J/mol×K	1249.34	Joback Method
cpg	1878.20	J/mol×K	1294.40	Joback Method
cpg	1894.33	J/mol×K	1339.46	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=C1561757&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

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