Disulfide, diheptyl

Other names:	8,9-Dithiahexadecane
	Diheptyl disulfide
	Heptyl disulfide
	di-n-Heptyl disulfide
	diheptyl disulphide
	n-Heptyl disulfide
Inchi:	InChI=1S/C14H30S2/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3-14H2,1-2H3
InchiKey:	IFGAFLQUAVLERP-UHFFFAOYSA-N
Formula:	C14H30S2
SMILES:	CCCCCCCSSCCCCCCC
Mol. weight [g/mol]:	262.52
CAS:	10496-16-9

Physical Properties

Property code	Value	Unit	Source
gf	133.24	kJ/mol	Joback Method
hf	-248.55	kJ/mol	Joback Method
hfus	40.28	kJ/mol	Joback Method
hvap	60.39	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	6.309		Crippen Method
mcvol	240.820	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
tb	657.28	K	Joback Method
tc	847.76	K	Joback Method
tf	316.34	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.14	J/mol×K	657.28	Joback Method
cpg	661.35	J/mol×K	689.03	Joback Method
cpg	678.66	J/mol×K	720.77	Joback Method

cpg	695.08	J/mol×K	752.52	Joback Method
cpg	710.63	J/mol×K	784.27	Joback Method
cpg	725.34	J/mol×K	816.01	Joback Method
cpg	739.21	J/mol×K	847.76	Joback Method
hvapt	69.80	kJ/mol	544.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46720e+01
Coeff. B	-4.95320e+03
Coeff. C	-1.06243e+02
Temperature range (K), min.	450.59
Temperature range (K), max.	635.40

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=C10496169&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume