Octane, 1,1'-thiobis-

Other names:	1-(1-Octylthio)octane
	1-(Octylsulfanyl)octane
	9-Thiaheptadecane
	Bis(1-octyl) sulfide
	Di-n-octyl sulfide
	Di-n-octyl thioether
	Dioctyl sulfide
	Dioctyl thioether
	NSC 65459
	Octyl sulfide
	dioctyl sulphide
	n-Octyl sulfide
Inchi:	InChI=1S/C16H34S/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h3-16H2,1-2H3
InchiKey:	LOXRGHGHQYWXJK-UHFFFAOYSA-N
Formula:	C16H34S
SMILES:	CCCCCCCCSCCCCCCCC
Mol. weight [g/mol]:	258.51
CAS:	2690-08-6

Physical Properties

Property code	Value	Unit	Source
gf	116.96	kJ/mol	Joback Method
hf	-331.70	kJ/mol	Joback Method
hfus	41.33	kJ/mol	Joback Method
hvap	95.00 ± 11.00	kJ/mol	NIST Webbook
log10ws	-6.40		Crippen Method
logp	6.441		Crippen Method
mcvol	252.650	ml/mol	McGowan Method
pc	1800.00 ± 200.00	kPa	NIST Webbook
rhoc	231.10 ± 14.99	kg/m3	NIST Webbook
rinpol	1892.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook

ripol	2048.00		NIST Webbook
ripol	2048.00		NIST Webbook
tb	634.26	K	Joback Method
tc	780.00 ± 6.00	K	NIST Webbook
tf	304.48	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.17	J/mol×K	634.26	Joback Method
cpg	704.36	J/mol×K	663.18	Joback Method
cpg	722.70	J/mol×K	692.10	Joback Method
cpg	740.22	J/mol×K	721.02	Joback Method
cpg	756.94	J/mol×K	749.94	Joback Method
cpg	772.88	J/mol×K	778.86	Joback Method
cpg	788.06	J/mol×K	807.78	Joback Method
hvapt	71.60	kJ/mol	388.50	NIST Webbook
hvapt	72.00 ± 0.60	kJ/mol	507.50	NIST Webbook
hvapt	67.80 ± 0.50	kJ/mol	507.50	NIST Webbook
hvapt	63.70 ± 0.60	kJ/mol	507.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54362e+01
Coeff. B	-5.19078e+03
Coeff. C	-1.05078e+02

Temperature range (K), min.	447.74
Temperature range (K), max.	617.76

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2690086&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume