DIOCTYL DISULPHIDE

Other names:	9,10-Dithiaoctadecane
	Bis(1-octyl) disulfide
	Diheptyl disulfide
	Dioctyl disulfide
	Disulfide, dioctyl
	Octyl disulfide
	di-n-Octyl disulfide
	n-Octyl disulfide
Inchi:	InChI=1S/C16H34S2/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h3-16H2,1-2H3
InchiKey:	AROCLDYPZXMJPW-UHFFFAOYSA-N
Formula:	C16H34S2
SMILES:	CCCCCCCCSSCCCCCCCC
Mol. weight [g/mol]:	290.58
CAS:	822-27-5

Physical Properties

Property code	Value	Unit	Source
af	0.7442		Cheméo Relay (1.0)
gf	150.08	kJ/mol	Joback Method
hf	-329.55	kJ/mol	Cheméo Relay (1.0)
hfus	45.46	kJ/mol	Joback Method
hvap	94.62	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-7.27		Cheméo Relay (1.0)
logp	7.089		Crippen Method
mcvol	269.000	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
tb	607.16	K	Cheméo Relay (1.0)
tc	779.86	K	Cheméo Relay (1.0)
tf	278.33	K	Cheméo Relay (1.0)
vc	1.036	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.36	J/mol×K	703.04	Joback Method
cpg	774.24	J/mol×K	734.32	Joback Method
cpg	792.15	J/mol×K	765.60	Joback Method
cpg	809.12	J/mol×K	796.89	Joback Method
cpg	825.17	J/mol×K	828.17	Joback Method
cpg	840.33	J/mol×K	859.45	Joback Method
cpg	854.61	J/mol×K	890.73	Joback Method
hvapt	73.90	kJ/mol	567.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46108e+01
Coeff. B	-5.12127e+03
Coeff. C	-1.13276e+02
Temperature range (K), min.	470.83
Temperature range (K), max.	663.99

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C822275&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor

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
ie:	Ionization energy
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