Decyl sulfide

Other names:	11-Thiaheneicosane
	Decane, 1,1'-thiobis-
	Didecyl sulfide
	di-n-Decyl sulfide
	didecyl sulphide
	n-Decyl sulfide
Inchi:	InChI=1S/C20H42S/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h3-20H2,1
InchiKey:	RKYMVQJWYYOIJB-UHFFFAOYSA-N
Formula:	C20H42S
SMILES:	CCCCCCCCCCSCCCCCCCCCC
Mol. weight [g/mol]:	314.61
CAS:	693-83-4

Physical Properties

Property code	Value	Unit	Source
gf	150.64	kJ/mol	Joback Method
hf	-414.26	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	66.93	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	8.001		Crippen Method
mcvol	309.010	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2281.00		NIST Webbook
tb	725.78	K	Joback Method
tc	900.07	K	Joback Method
tf	300.40 ± 2.00	K	NIST Webbook
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.76	J/mol×K	725.78	Joback Method
cpg	939.38	J/mol×K	754.83	Joback Method
cpg	959.02	J/mol×K	783.88	Joback Method
cpg	977.73	J/mol×K	812.92	Joback Method
cpg	995.53	J/mol×K	841.97	Joback Method
cpg	1012.46	J/mol×K	871.02	Joback Method
cpg	1028.53	J/mol×K	900.07	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50751e+01
Coeff. B	-5.42985e+03
Coeff. C	-1.18144e+02
Temperature range (K), min.	485.34
Temperature range (K), max.	674.27

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C693834&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume