n-Dodecylmethyl sulfide

Other names:	1-(Methylsulfanyl)dodecane
	1-Methylthiododecane
	2-Thiatetradecane
	Dodecane, 1-(methylthio)-
	Dodecyl methyl sulfide
	Dodecyl methyl sulphide
	Methyl lauryl sulfide
	Methyl n-dodecyl sulfide
	NSC 87889
	Sulfide, dodecyl methyl
Inchi:	InChI=1S/C13H28S/c1-3-4-5-6-7-8-9-10-11-12-13-14-2/h3-13H2,1-2H3
InchiKey:	KJWHJDGMOQJLGF-UHFFFAOYSA-N
Formula:	C13H28S
SMILES:	CCCCCCCCCCCCSC
Mol. weight [g/mol]:	216.43
CAS:	3698-89-3

Physical Properties

Property code	Value	Unit	Source
gf	91.70	kJ/mol	Joback Method
hf	-269.78	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	5.270		Crippen Method
mcvol	210.380	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1858.00		NIST Webbook
tb	565.62	K	Joback Method
tc	742.46	K	Joback Method
tf	270.67	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.41	J/mol×K	565.62	Joback Method
cpg	541.20	J/mol×K	595.09	Joback Method
cpg	558.24	J/mol×K	624.57	Joback Method
cpg	574.54	J/mol×K	654.04	Joback Method
cpg	590.11	J/mol×K	683.52	Joback Method
cpg	604.99	J/mol×K	712.99	Joback Method
cpg	619.17	J/mol×K	742.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61829e+01
Coeff. B	-5.14627e+03
Coeff. C	-9.50150e+01
Temperature range (K), min.	418.78
Temperature range (K), max.	568.39

Sources

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=C3698893&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume