

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
af	0.6231		Cheméo Relay (1.0)
gf	91.70	kJ/mol	Joback Method
hf	-286.63	kJ/mol	Cheméo Relay (1.0)
hfus	33.56	kJ/mol	Joback Method
hvap	77.46	kJ/mol	Cheméo Relay (1.0)
ie	8.67	eV	Cheméo Relay (1.0)
log10ws	-6.24		Cheméo Relay (1.0)
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	550.65	K	Cheméo Relay (1.0)
tc	730.74	K	Cheméo Relay (1.0)
tf	287.44	K	Cheméo Relay (1.0)

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	$\ln(P_{vp}) = A + B/(T + C)$
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

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>

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:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3698893&Units=SI>

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
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
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

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