1-Dodecanethiol

Other names:	1-Dodecyl mercaptan
	1-Dodecylthiol
	1-Mercaptododecane
	Dodecane-1-thiol
	Dodecanethiol-(1)
	Dodecyl mercaptan
	Dodecylthiol
	Lauryl mercaptan
	N-DODECANETHIOL
	N-LAURYL MERCAPTAN
	NCI-C60935
	NSC 814
	Pennfloat M
	Pennfloat S
	n-Dodecyl mercaptan
	n-Dodecylthiol
Inchi:	InChI=1S/C12H26S/c1-2-3-4-5-6-7-8-9-10-11-12-13/h13H,2-12H2,1H3
InchiKey:	WNAHIZMDSQCWRP-UHFFFAOYSA-N
Formula:	C12H26S
SMILES:	CCCCCCCCCCCCS
Mol. weight [g/mol]:	202.40
CAS:	112-55-0

Physical Properties

Property code	Value	Unit	Source
gf	79.55	kJ/mol	Joback Method
hf	-252.53	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	49.04	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.837		Crippen Method
mcvol	196.290	ml/mol	McGowan Method
pc	1810.00	kPa	Critical Point and Vapor Pressure Measurements for Seven Compounds by a Low Residence Time Flow Method
rinpol	1536.00		NIST Webbook

rinpol	1520.00		NIST Webbook
rinpol	1536.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1773.00		NIST Webbook
tb	547.70	K	NIST Webbook
tc	715.23	K	Joback Method
tf	261.46	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.06	J/mol×K	536.82	Joback Method
cpg	486.24	J/mol×K	566.56	Joback Method
cpg	502.67	J/mol×K	596.29	Joback Method
cpg	518.40	J/mol×K	626.03	Joback Method
cpg	533.42	J/mol×K	655.76	Joback Method
cpg	547.77	J/mol×K	685.50	Joback Method
cpg	561.47	J/mol×K	715.23	Joback Method
cpl	442.81	J/mol×K	300.00	NIST Webbook
hvapt	62.00	kJ/mol	500.50	NIST Webbook
rfi	1.45860		298.20	Solubility and Tie Line Data of the Water - Phosphoric Acid Solvents at T = (303.2 and 313.2) K: An Experimental and Correlational Study

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55265e+01
Coeff. B	-4.95533e+03
Coeff. C	-9.34240e+01
Temperature range (K), min.	418.60
Temperature range (K), max.	578.53

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.42315e+02
Coeff. B	-1.35158e+04
Coeff. C	-1.83538e+01
Coeff. D	9.03950e-06
Temperature range (K), min.	265.15
Temperature range (K), max.	724.00

Sources

Solubility and Tie Line Data of the Water - Phosphoric Acid - Solvents at T = (303.2 and 313.2) K: An Experimental and Correlational Study:	https://www.doi.org/10.1016/j.tca.2013.02.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C112550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Critical Point and Vapor Pressure Measurements for Seven Compounds by a Low Residence Time Flow Method:	https://www.doi.org/10.1021/je060088h
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1850
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1850.mol

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
rfi:	Refractive Index
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