

2-Undecanethiol, 2-methyl-

Other names:	1,1-Dimethyl-decyl-mercaptan 2-Methyl-2-undecanethiol 2-Methylundecane-2-thiol 2-Methylundecyl-2-thiol
Inchi:	InChI=1S/C12H26S/c1-4-5-6-7-8-9-10-11-12(2,3)13/h13H,4-11H2,1-3H3
InchiKey:	FRQQKWGDKVGLFI-UHFFFAOYSA-N
Formula:	C12H26S
SMILES:	CCCCCCCCC(C)(C)S
Mol. weight [g/mol]:	202.40
CAS:	10059-13-9

Physical Properties

Property code	Value	Unit	Source
gf	82.39	kJ/mol	Joback Method
hf	-261.28	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	47.75	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.835		Crippen Method
mcvol	196.290	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
tb	533.59	K	Joback Method
tc	722.19	K	Joback Method
tf	263.88	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.83	J/mol×K	533.59	Joback Method
cpg	490.12	J/mol×K	565.02	Joback Method
cpg	507.49	J/mol×K	596.46	Joback Method
cpg	523.96	J/mol×K	627.89	Joback Method
cpg	539.59	J/mol×K	659.32	Joback Method

cpg	554.41	J/mol×K	690.75	Joback Method
cpg	568.46	J/mol×K	722.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40041e+01
Coeff. B	-4.28724e+03
Coeff. C	-8.69190e+01
Temperature range (K), min.	399.48
Temperature range (K), max.	580.12

Sources

The Yaws Handbook of Vapor Pressure: Crippen Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10059139&Units=SI

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

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

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