

1-Undecanethiol

Other names:	1-Undecylthiol Undecyl mercaptan
Inchi:	InChI=1S/C11H24S/c1-2-3-4-5-6-7-8-9-10-11-12/h12H,2-11H2,1H3
InchiKey:	CCIDWXHLGNEQSL-UHFFFAOYSA-N
Formula:	C11H24S
SMILES:	CCCCCCCCCCCS
Mol. weight [g/mol]:	188.37
CAS:	5332-52-5

Physical Properties

Property code	Value	Unit	Source
gf	71.13	kJ/mol	Joback Method
hf	-231.89	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	46.82	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.447		Crippen Method
mcvol	182.200	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1673.00		NIST Webbook
tb	513.94	K	Joback Method
tc	694.08	K	Joback Method
tf	250.19	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.16	J/molxK	513.94	Joback Method
cpg	436.67	J/molxK	543.96	Joback Method

cpg	452.47	J/mol×K	573.99	Joback Method
cpg	467.58	J/mol×K	604.01	Joback Method
cpg	482.02	J/mol×K	634.03	Joback Method
cpg	495.82	J/mol×K	664.05	Joback Method
cpg	508.99	J/mol×K	694.08	Joback Method
hvapt	59.30	kJ/mol	484.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58676e+01
Coeff. B	-4.92636e+03
Coeff. C	-8.86430e+01
Temperature range (K), min.	404.84
Temperature range (K), max.	555.32

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

KDB:

<https://www.thermo.com/files/research/kdb/mol/mol1849.mol>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5332525&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

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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