

1-Pentadecanethiol

Other names:	pentadecane-1-thiol
Inchi:	InChI=1S/C15H32S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16/h16H,2-15H2,1H3
InchiKey:	IGMQODZGDORXEN-UHFFFAOYSA-N
Formula:	C15H32S
SMILES:	CCCCCCCCCCCCCCCCS
Mol. weight [g/mol]:	244.48
CAS:	25276-70-4

Physical Properties

Property code	Value	Unit	Source
gf	104.81	kJ/mol	Joback Method
hf	-314.45	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	6.007		Crippen Method
mcvol	238.560	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
tb	605.46	K	Joback Method
tc	779.70	K	Joback Method
tf	295.27	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.52	J/mol×K	605.46	Joback Method
cpg	644.27	J/mol×K	634.50	Joback Method
cpg	662.19	J/mol×K	663.54	Joback Method
cpg	679.33	J/mol×K	692.58	Joback Method
cpg	695.69	J/mol×K	721.62	Joback Method
cpg	711.31	J/mol×K	750.66	Joback Method
cpg	726.22	J/mol×K	779.70	Joback Method
hvapt	69.80	kJ/mol	544.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58161e+01
Coeff. B	-5.42327e+03
Coeff. C	-1.06243e+02
Temperature range (K), min.	455.49
Temperature range (K), max.	622.52

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=C25276704&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
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
tb:	Normal Boiling Point Temperature

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

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