

1-Tridecanethiol

Other names:	Tridecyl mercaptan tridecane-1-thiol
Inchi:	InChI=1S/C13H28S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h14H,2-13H2,1H3
InchiKey:	IPBROXKVGHZHJV-UHFFFAOYSA-N
Formula:	C13H28S
SMILES:	CCCCCCCCCCCCCS
Mol. weight [g/mol]:	216.43
CAS:	19484-26-5

Physical Properties

Property code	Value	Unit	Source
gf	87.97	kJ/mol	Joback Method
hf	-273.17	kJ/mol	Joback Method
hfus	33.47	kJ/mol	Joback Method
hvap	51.27	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.227		Crippen Method
mcvol	210.380	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
tb	559.70	K	Joback Method
tc	736.52	K	Joback Method
tf	272.73	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.65	J/mol×K	559.70	Joback Method
cpg	537.42	J/mol×K	589.17	Joback Method
cpg	554.42	J/mol×K	618.64	Joback Method
cpg	570.67	J/mol×K	648.11	Joback Method
cpg	586.20	J/mol×K	677.58	Joback Method
cpg	601.03	J/mol×K	707.05	Joback Method
cpg	615.19	J/mol×K	736.52	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58669e+01
Coeff. B	-5.19783e+03
Coeff. C	-9.79310e+01
Temperature range (K), min.	431.57
Temperature range (K), max.	590.36

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/ci990307l>

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=C19484265&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
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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