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
af	0.7062		Cheméo Relay (1.0)
gf	87.97	kJ/mol	Joback Method
hf	-285.53	kJ/mol	Cheméo Relay (1.0)
hfus	33.47	kJ/mol	Joback Method
hvap	79.46	kJ/mol	Cheméo Relay (1.0)
ie	9.24	eV	Cheméo Relay (1.0)
log10ws	-6.42		Cheméo Relay (1.0)
logp	5.227		Crippen Method
mcvol	210.380	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
tb	555.78	K	Cheméo Relay (1.0)
tc	731.19	K	Cheméo Relay (1.0)
tf	289.96	K	Cheméo Relay (1.0)
vc	0.827	m3/kmol	Cheméo Relay (1.0)

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
hvapt	64.70	kJ/mol	515.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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=C19484265&Units=SI

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

Legend

af: Acentric Factor

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

ie:	Ionization energy
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