Octacosanol

Other names:	1-Octacosanol
	Cluytyl alcohol
	Montanyl alcohol
	Octacosyl alcohol
	n-Octacosanol
	octacosan-1-ol
Inchi:	InChI=1S/C28H58O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-
InchiKey:	CNNRPFQICPFDPO-UHFFFAOYSA-N
Formula:	C28H58O
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	410.76
CAS:	557-61-9

Physical Properties

Property code	Value	Unit	Source
gf	48.06	kJ/mol	Joback Method
hf	-773.48	kJ/mol	Joback Method
hfus	108.44	kJ/mol	Solubility of commercial octacosanol in organic solvents and their correlation by thermodynamic models at different temperatures
hvap	94.60	kJ/mol	Joback Method
log10ws	-10.81		Crippen Method
logp	10.141		Crippen Method
mcvol	411.250	ml/mol	McGowan Method
pc	687.45	kPa	Joback Method
rinpol	3118.10		NIST Webbook
rinpol	3110.60		NIST Webbook
rinpol	3110.60		NIST Webbook
rinpol	3120.00		NIST Webbook
tb	932.22	K	Joback Method
tc	1160.42	K	Joback Method
tf	466.14	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1437.04	J/mol×K	932.22	Joback Method
cpg	1552.70	J/mol×K	1122.38	Joback Method
cpg	1532.39	J/mol×K	1084.35	Joback Method
cpg	1510.78	J/mol×K	1046.32	Joback Method
cpg	1487.76	J/mol×K	1008.29	Joback Method
cpg	1463.22	J/mol×K	970.25	Joback Method
cpg	1571.81	J/mol×K	1160.42	Joback Method
dvisc	0.0000044	Pa×s	932.22	Joback Method
dvisc	0.0000070	Pa×s	854.54	Joback Method
dvisc	0.0000121	Pa×s	776.86	Joback Method
dvisc	0.0000235	Pa×s	699.18	Joback Method
dvisc	0.0000541	Pa×s	621.50	Joback Method
dvisc	0.0001581	Pa×s	543.82	Joback Method
dvisc	0.0006608	Pa×s	466.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52464e+01
Coeff. B	-6.30015e+03
Coeff. C	-1.41032e+02
Temperature range (K), min.	562.20
Temperature range (K), max.	775.18

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of commercial octacosanol in organic solvents and their correlation by thermodynamic models at different temperatures:	https://www.doi.org/10.1016/j.jct.2017.02.025
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=C557619&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume