1-Eicosanol, 2-hexadecyl-

Other names: Pentatriacontane, 17-(hydroxymethyl)-
2-hexadecylicosanol
Inchi: InChI=1S/C36H74O/c1-3-5-7-9-11-13-15-17-19-20-22-24-26-28-30-32-34-36(35-37)33-3
InchiKey: JQJGGMZIMBGQQY-UHFFFAOYSA-N
Formula: C36H74O
SMILES: CCCCCCCCCCCCCCCCCCC(CO)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 522.97
CAS: 17658-63-8

Physical Properties

Property code	Value	Unit	Source
gf	112.98	kJ/mol	Joback Method
hf	-943.88	kJ/mol	Joback Method
hfus	89.56	kJ/mol	Joback Method
hvap	112.02	kJ/mol	Joback Method
log10ws	-13.91		Crippen Method
logp	13.118		Crippen Method
mcvol	523.970	ml/mol	McGowan Method
pc	477.98	kPa	Joback Method
rinpol	3782.00		NIST Webbook
tb	1114.82	K	Joback Method
tc	1487.90	K	Joback Method
tf	541.30	K	Joback Method
vc	2.064	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1980.02	J/mol×K	1114.82	Joback Method
cpg	2019.41	J/mol×K	1177.00	Joback Method
cpg	2055.23	J/mol×K	1239.18	Joback Method
cpg	2088.09	J/mol×K	1301.36	Joback Method
cpg	2118.60	J/mol×K	1363.54	Joback Method
cpg	2147.39	J/mol×K	1425.72	Joback Method

cpg	2175.06	J/mol×K	1487.90	Joback Method
dvisc	0.0001609	Pa×s	541.30	Joback Method
dvisc	0.0000354	Pa×s	636.89	Joback Method
dvisc	0.0000116	Pa×s	732.47	Joback Method
dvisc	0.0000049	Pa×s	828.06	Joback Method
dvisc	0.0000025	Pa×s	923.65	Joback Method
dvisc	0.0000014	Pa×s	1019.23	Joback Method
dvisc	0.0000009	Pa×s	1114.82	Joback Method

Sources

Crippen Method:	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=C17658638&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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