

Octacosyl pentyl ether

Inchi:	InChI=1S/C33H68O/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey:	OBVCNZKHGXGUJR-UHFFFAOYSA-N
Formula:	C33H68O
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCOCCCCC
Mol. weight [g/mol]:	480.89

Physical Properties

Property code	Value	Unit	Source
gf	121.98	kJ/mol	Joback Method
hf	-856.67	kJ/mol	Joback Method
hfus	82.41	kJ/mol	Joback Method
hvap	91.46	kJ/mol	Joback Method
log10ws	-12.72		Crippen Method
logp	12.356		Crippen Method
mvol	481.700	ml/mol	McGowan Method
pc	515.83	kPa	Joback Method
rinpol	3369.00		NIST Webbook
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tb	976.86	K	Joback Method
tc	1229.09	K	Joback Method
tf	483.90	K	Joback Method
vc	1.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1722.96	J/molxK	976.86	Joback Method
cpg	1753.98	J/molxK	1018.90	Joback Method
cpg	1782.66	J/molxK	1060.94	Joback Method
cpg	1809.15	J/molxK	1102.97	Joback Method
cpg	1833.60	J/molxK	1145.01	Joback Method
cpg	1856.14	J/molxK	1187.05	Joback Method
cpg	1876.92	J/molxK	1229.09	Joback Method
dvisc	0.0004509	Paxs	483.90	Joback Method

dvisc	0.0001560	Paxs	566.06	Joback Method
dvisc	0.0000706	Paxs	648.22	Joback Method
dvisc	0.0000382	Paxs	730.38	Joback Method
dvisc	0.0000234	Paxs	812.54	Joback Method
dvisc	0.0000157	Paxs	894.70	Joback Method
dvisc	0.0000112	Paxs	976.86	Joback Method

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=U406424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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