octyl hexacosanoate

Inchi: InChI=1S/C34H68O2/c1-3-5-7-9-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-
InchiKey: DDMCRMVINUTGIA-UHFFFAOYSA-N
Formula: C34H68O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 508.90

Physical Properties

Property code	Value	Unit	Source
gf	1.48	kJ/mol	Joback Method
hf	-989.89	kJ/mol	Joback Method
hfus	86.60	kJ/mol	Joback Method
hvap	100.43	kJ/mol	Joback Method
log10ws	-12.92		Crippen Method
logp	12.272		Crippen Method
mcvol	497.360	ml/mol	McGowan Method
pc	508.18	kPa	Joback Method
rinpol	3562.26		NIST Webbook
tb	1053.61	K	Joback Method
tc	1347.22	K	Joback Method
tf	545.10	K	Joback Method
vc	1.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1818.58	J/mol×K	1053.61	Joback Method
cpg	1849.65	J/mol×K	1102.55	Joback Method
cpg	1877.82	J/mol×K	1151.48	Joback Method
cpg	1903.31	J/mol×K	1200.42	Joback Method
cpg	1926.37	J/mol×K	1249.35	Joback Method
cpg	1947.21	J/mol×K	1298.29	Joback Method
cpg	1966.09	J/mol×K	1347.22	Joback Method
dvisc	0.0002762	Pa×s	545.10	Joback Method
dvisc	0.0001060	Pa×s	629.85	Joback Method

dvisc	0.0000510	Pa×s	714.60	Joback Method
dvisc	0.0000287	Pa×s	799.36	Joback Method
dvisc	0.0000180	Pa×s	884.11	Joback Method
dvisc	0.0000123	Pa×s	968.86	Joback Method
dvisc	0.0000089	Pa×s	1053.61	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=R437953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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