

hexadecyl lactate

Inchi:	InChI=1S/C19H38O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-19(21)18(2)20/h18,2
InchiKey:	WUKXMJCZWYUIRZ-UHFFFAOYSA-N
Formula:	C19H38O3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(C)O
Mol. weight [g/mol]:	314.50
CAS:	35274-05-6

Physical Properties

Property code	Value	Unit	Source
gf	-264.08	kJ/mol	Joback Method
hf	-837.80	kJ/mol	Joback Method
hfus	48.32	kJ/mol	Joback Method
hvap	83.33	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.392		Crippen Method
mcvol	291.880	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
tb	802.15	K	Joback Method
tc	982.84	K	Joback Method
tf	314.00 ± 2.00	K	NIST Webbook
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.10	J/molxK	982.84	Joback Method
cpg	1005.86	J/molxK	952.72	Joback Method
cpg	991.80	J/molxK	922.61	Joback Method
cpg	976.88	J/molxK	892.49	Joback Method
cpg	961.08	J/molxK	862.38	Joback Method
cpg	944.38	J/molxK	832.26	Joback Method
cpg	926.75	J/molxK	802.15	Joback Method
dvisc	0.0015575	Paxs	421.87	Joback Method
dvisc	0.0000135	Paxs	802.15	Joback Method

dvisc	0.0000212	Paxs	738.77	Joback Method
dvisc	0.0000363	Paxs	675.39	Joback Method
dvisc	0.0000694	Paxs	612.01	Joback Method
dvisc	0.0001540	Paxs	548.63	Joback Method
dvisc	0.0004210	Paxs	485.25	Joback Method
hvapt	90.50	kJ/mol	480.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35274056&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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