Hexyl laurate

Other names: hexyl dodecanoate
Inchi: InChI=1S/C18H36O2/c1-3-5-7-9-10-11-12-13-14-16-18(19)20-17-15-8-6-4-2/h3-17H2,1-2
InchiKey: CMBYOWLFQAFZCP-UHFFFAOYSA-N
Formula: C18H36O2
SMILES: CCCCCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 284.48
CAS: 34316-64-8

Physical Properties

Property code	Value	Unit	Source
gf	-133.24	kJ/mol	Joback Method
hf	-659.65	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	64.82	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	6.031		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
rinpol	1963.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	1983.20		NIST Webbook
rinpol	1983.20		NIST Webbook
tb	687.53	K	Joback Method
tc	855.83	K	Joback Method
tf	269.75 ± 3.00	K	NIST Webbook
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.92	J/mol×K	687.53	Joback Method
cpg	875.72	J/mol×K	827.78	Joback Method
cpg	860.14	J/mol×K	799.73	Joback Method
cpg	843.80	J/mol×K	771.68	Joback Method

cpg	826.65	J/mol×K	743.63	Joback Method
cpg	808.70	J/mol×K	715.58	Joback Method
cpg	890.54	J/mol×K	855.83	Joback Method
dvisc	0.0000953	Pa×s	687.53	Joback Method
dvisc	0.0001278	Pa×s	633.74	Joback Method
dvisc	0.0001809	Pa×s	579.95	Joback Method
dvisc	0.0002749	Pa×s	526.15	Joback Method
dvisc	0.0004595	Pa×s	472.36	Joback Method
dvisc	0.0008765	Pa×s	418.57	Joback Method
dvisc	0.0020226	Pa×s	364.78	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=C34316648&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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