Isovaleric acid, undecyl ester

Inchi: InChI=1S/C16H32O2/c1-4-5-6-7-8-9-10-11-12-13-18-16(17)14-15(2)3/h15H,4-14H2,1-3H
InchiKey: ITSQZEZOZHBTQN-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CCCCCCCCCCCOC(=O)CC(C)C
Mol. weight [g/mol]: 256.42

Physical Properties

Property code	Value	Unit	Source
gf	-152.52	kJ/mol	Joback Method
hf	-623.65	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	59.98	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	5.107		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
tb	641.33	K	Joback Method
tc	810.93	K	Joback Method
tf	327.24	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.23	J/mol×K	641.33	Joback Method
cpg	694.40	J/mol×K	669.60	Joback Method
cpg	711.78	J/mol×K	697.86	Joback Method
cpg	728.40	J/mol×K	726.13	Joback Method
cpg	744.26	J/mol×K	754.40	Joback Method
cpg	759.39	J/mol×K	782.67	Joback Method
cpg	773.80	J/mol×K	810.93	Joback Method
dvisc	0.0031617	Pa×s	327.24	Joback Method

dvisc	0.0012389	Pa×s	379.59	Joback Method
dvisc	0.0006092	Pa×s	431.94	Joback Method
dvisc	0.0003493	Pa×s	484.28	Joback Method
dvisc	0.0002232	Pa×s	536.63	Joback Method
dvisc	0.0001544	Pa×s	588.98	Joback Method
dvisc	0.0001135	Pa×s	641.33	Joback Method

Sources

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=U340259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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