1-Propoxypropan-2-yl 3,5,5-trimethylhexanoate

Inchi: InChI=1S/C15H30O3/c1-7-8-17-11-13(3)18-14(16)9-12(2)10-15(4,5)6/h12-13H,7-11H2,1

InchiKey: UWUZSZNNQJCARS-UHFFFAOYSA-N

Formula: C15H30O3

SMILES: CCCOCC(C)OC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 258.40

Physical Properties

Property code	Value	Unit	Source
gf	-265.54	kJ/mol	Joback Method
hf	-749.26	kJ/mol	Joback Method
hfus	24.12	kJ/mol	Joback Method
hvap	58.48	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.807		Crippen Method
mcvol	235.520	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	1521.00		NIST Webbook
rinpol	1521.00		NIST Webbook
tb	637.20	K	Joback Method
tc	817.10	K	Joback Method
tf	325.62	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.23	J/mol×K	637.20	Joback Method
cpg	672.61	J/mol×K	667.18	Joback Method
cpg	690.11	J/mol×K	697.17	Joback Method
cpg	706.74	J/mol×K	727.15	Joback Method
cpg	722.53	J/mol×K	757.14	Joback Method
cpg	737.50	J/mol×K	787.12	Joback Method
cpg	751.66	J/mol×K	817.10	Joback Method
dvisc	0.0035901	Pa×s	325.62	Joback Method

dvisc	0.0012334	Pa×s	377.55	Joback Method
dvisc	0.0005486	Pa×s	429.48	Joback Method
dvisc	0.0002907	Pa×s	481.41	Joback Method
dvisc	0.0001743	Pa×s	533.34	Joback Method
dvisc	0.0001144	Pa×s	585.27	Joback Method
dvisc	0.0000804	Pa×s	637.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378242&Units=SI
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

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