octyl 2-hydroxypropanoate

Inchi: InChI=1S/C11H22O3/c1-3-4-5-6-7-8-9-14-11(13)10(2)12/h10,12H,3-9H2,1-2H3
InchiKey: SFBIZPBTKROSDE-UHFFFAOYSA-N
Formula: C11H22O3
SMILES: CCCCCCCCOC(=O)C(C)O
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
gf	-331.44	kJ/mol	Joback Method
hf	-672.68	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-1.27		Aqueous Solubility Prediction Method
logp	2.271		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
tb	619.11	K	Joback Method
tc	788.09	K	Joback Method
tf	331.71	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.00	J/mol×K	619.11	Joback Method
cpg	492.23	J/mol×K	647.27	Joback Method
cpg	504.91	J/mol×K	675.44	Joback Method
cpg	517.04	J/mol×K	703.60	Joback Method
cpg	528.63	J/mol×K	731.76	Joback Method
cpg	539.68	J/mol×K	759.93	Joback Method
cpg	550.21	J/mol×K	788.09	Joback Method
dvisc	0.0077301	Pa×s	331.71	Joback Method
dvisc	0.0020635	Pa×s	379.61	Joback Method

dvisc	0.0007406	Pa×s	427.51	Joback Method
dvisc	0.0003267	Pa×s	475.41	Joback Method
dvisc	0.0001675	Pa×s	523.31	Joback Method
dvisc	0.0000960	Pa×s	571.21	Joback Method
dvisc	0.0000600	Pa×s	619.11	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume