3-hydroxy-2,2,4-trimethylpentyl isobutyrate

Other names: 2-methylpropanoic acid-3-hydroxy-2,4,4-trimethylpentyl ester
Inchi: InChI=1S/C12H24O3/c1-8(2)10(13)12(5,6)7-15-11(14)9(3)4/h8-10,13H,7H2,1-6H3
InchiKey: DAFHKNAQFPVRKR-UHFFFAOYSA-N
Formula: C12H24O3
SMILES: CC(C)C(=O)OCC(C)(C)C(O)C(C)C
Mol. weight [g/mol]: 216.32
CAS: 77-68-9

Physical Properties

Property code	Value	Unit	Source
gf	-325.06	kJ/mol	Joback Method
hf	-712.63	kJ/mol	Joback Method
hfus	15.73	kJ/mol	Joback Method
hvap	65.68	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.229		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1380.00		NIST Webbook
rinpol	1365.20		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1380.00		NIST Webbook
tb	637.88	K	Joback Method
tc	818.75	K	Joback Method
tf	315.40	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.41	J/mol×K	637.88	Joback Method
cpg	601.10	J/mol×K	788.60	Joback Method
cpg	589.17	J/mol×K	758.46	Joback Method
cpg	576.56	J/mol×K	728.31	Joback Method

cpg	563.25	J/mol×K	698.17	Joback Method
cpg	549.20	J/mol×K	668.02	Joback Method
cpg	612.37	J/mol×K	818.75	Joback Method
dvisc	0.0000380	Pa×s	637.88	Joback Method
dvisc	0.0000666	Pa×s	584.13	Joback Method
dvisc	0.0001306	Pa×s	530.39	Joback Method
dvisc	0.0002981	Pa×s	476.64	Joback Method
dvisc	0.0008392	Pa×s	422.89	Joback Method
dvisc	0.0031940	Pa×s	369.15	Joback Method
dvisc	0.0191716	Pa×s	315.40	Joback Method

Sources

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=C77689&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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