2-Methyl-1-(1,1-dimethylethyl)-2-methylpropanoic acid, 1,3-propanediyl ester

Inchi: InChI=1S/C15H28O4/c1-9(2)13(16)18-11(5)12(15(6,7)8)19-14(17)10(3)4/h9-12H,1-8H3
InchiKey: FERSOBASMASJSG-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CC(C)C(=O)OC(C)C(OC(=O)C(C)C)C(C)(C)C
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-399.34	kJ/mol	Joback Method
hf	-872.40	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	64.45	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.188		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	1603.00		NIST Webbook
tb	690.19	K	Joback Method
tc	883.12	K	Joback Method
tf	345.55	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.51	J/mol×K	690.19	Joback Method
cpg	699.09	J/mol×K	722.34	Joback Method
cpg	715.67	J/mol×K	754.50	Joback Method
cpg	731.28	J/mol×K	786.65	Joback Method
cpg	745.94	J/mol×K	818.81	Joback Method
cpg	759.67	J/mol×K	850.96	Joback Method
cpg	772.50	J/mol×K	883.12	Joback Method
dvisc	0.0040359	Pa×s	345.55	Joback Method
dvisc	0.0012450	Pa×s	402.99	Joback Method

dvisc	0.0005150	Pa×s	460.43	Joback Method
dvisc	0.0002591	Pa×s	517.87	Joback Method
dvisc	0.0001496	Pa×s	575.31	Joback Method
dvisc	0.0000954	Pa×s	632.75	Joback Method
dvisc	0.0000655	Pa×s	690.19	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=R73616&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