Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester

Othernames: 2,2,4-trimethyl-3-carboxyisopropylpentanoic acid isobutyl ester
Inchi: InChI=1S/C16H30O4/c1-10(2)9-19-15(18)16(7,8)13(11(3)4)14(17)20-12(5)6/h10-13H,9H
InchiKey: JIYRKVLLOCBJHR-UHFFFAOYSA-N
Formula: C16H30O4
SMILES: CC(C)COC(=O)C(C)(C)C(C(=O)OC(C)C)C(C)C
Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-390.92	kJ/mol	Joback Method
hf	-893.04	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	66.67	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.436		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	1581.00		NIST Webbook
tb	713.07	K	Joback Method
tc	904.59	K	Joback Method
tf	356.82	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.61	J/mol×K	713.07	Joback Method
cpg	755.46	J/mol×K	744.99	Joback Method
cpg	772.29	J/mol×K	776.91	Joback Method
cpg	788.13	J/mol×K	808.83	Joback Method
cpg	802.99	J/mol×K	840.75	Joback Method
cpg	816.90	J/mol×K	872.67	Joback Method
cpg	829.89	J/mol×K	904.59	Joback Method
dvisc	0.0034893	Pa×s	356.82	Joback Method

dvisc	0.0010748	Pa×s	416.20	Joback Method
dvisc	0.0004442	Pa×s	475.57	Joback Method
dvisc	0.0002234	Pa×s	534.95	Joback Method
dvisc	0.0001289	Pa×s	594.32	Joback Method
dvisc	0.0000822	Pa×s	653.70	Joback Method
dvisc	0.0000565	Pa×s	713.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U140775&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