Propanoic acid, 2-methyl-, 1-methyl-1-(4-methyl-3-cyclohexen-1-yl)ethyl ester

Othernames: «alpha»-Terpinyl ester of isobutanoic acid
Terpinyl isobutyrate
1-Methyl-1-(4-methyl-3-cyclohexen-1-yl)ethyl 2-methylpropanoate
«alpha»-Terpinyl isobutyrate
p-Menth-1-en-8-yl isobutyrate
1-methyl-1-(4-methylcyclohex-3-enyl)ethyl isobutyrate

Inchi: InChI=1S/C14H24O2/c1-10(2)13(15)16-14(4,5)12-8-6-11(3)7-9-12/h6,10,12H,7-9H2,1-5H

InchiKey: SMQUXKIIXFOJKI-UHFFFAOYSA-N

Formula: C14H24O2

SMILES: CC1=CCC(C(C)(C)OC(=O)C(C)C)CC1

Mol. weight [g/mol]: 224.34

CAS: 7774-65-4

Physical Properties

Property code	Value	Unit	Source
gf	-121.74	kJ/mol	Joback Method
hf	-490.49	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	55.61	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.711		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1462.40		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1462.40		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1751.00		NIST Webbook
tb	616.03	K	Joback Method
tc	827.74	K	Joback Method
tf	327.78	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.93	J/mol×K	616.03	Joback Method
cpg	562.04	J/mol×K	651.32	Joback Method
cpg	580.94	J/mol×K	686.60	Joback Method
cpg	598.66	J/mol×K	721.89	Joback Method
cpg	615.25	J/mol×K	757.17	Joback Method
cpg	630.74	J/mol×K	792.46	Joback Method
cpg	645.18	J/mol×K	827.74	Joback Method
dvisc	0.0033910	Pa×s	327.78	Joback Method
dvisc	0.0014087	Pa×s	375.82	Joback Method
dvisc	0.0007141	Pa×s	423.86	Joback Method
dvisc	0.0004157	Pa×s	471.90	Joback Method
dvisc	0.0002675	Pa×s	519.95	Joback Method
dvisc	0.0001854	Pa×s	567.99	Joback Method
dvisc	0.0001361	Pa×s	616.03	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7774654&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

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