«alpha»-Terpinyl isovalerate

Other names:	Terpinyl iso-valerate
	«alpha»-Terpinyl isopentanoate
	n-Terpinenyl ester of isopentanoic acid
	Isovaleric acid, p-menth-1-en-8-yl ester
	«alpha»-Terpenyl isovalerate
	Butanoic acid, 3-methyl-, 1-methyl-1-(4-methyl-3-cyclohexen-1-yl)ethyl ester
	2-(4-methyl-1-cyclohex-3-enyl)propan-2-yl 3-methylbutanoate
Inchi:	InChI=1S/C15H26O2/c1-11(2)10-14(16)17-15(4,5)13-8-6-12(3)7-9-13/h6,11,13H,7-10H2
InchiKey:	XRADSECIALQFFY-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	CC1=CCC(C(C)(C)OC(=O)CC(C)C)CC1
Mol. weight [g/mol]:	238.37
CAS:	1142-85-4

Physical Properties

Property code	Value	Unit	Source
gf	-113.32	kJ/mol	Joback Method
hf	-511.13	kJ/mol	Joback Method
hfus	19.12	kJ/mol	Joback Method
hvap	57.84	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.101		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	1498.00		NIST Webbook
rinpol	1501.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1858.00		NIST Webbook
tb	638.91	K	Joback Method
tc	847.30	K	Joback Method
tf	339.05	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.79	J/mol×K	638.91	Joback Method
cpg	616.17	J/mol×K	673.64	Joback Method
cpg	635.33	J/mol×K	708.37	Joback Method
cpg	653.30	J/mol×K	743.10	Joback Method
cpg	670.12	J/mol×K	777.84	Joback Method
cpg	685.85	J/mol×K	812.57	Joback Method
cpg	700.51	J/mol×K	847.30	Joback Method
dvisc	0.0031021	Pa×s	339.05	Joback Method
dvisc	0.0012749	Pa×s	389.03	Joback Method
dvisc	0.0006416	Pa×s	439.00	Joback Method
dvisc	0.0003715	Pa×s	488.98	Joback Method
dvisc	0.0002381	Pa×s	538.96	Joback Method
dvisc	0.0001645	Pa×s	588.93	Joback Method
dvisc	0.0001205	Pa×s	638.91	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1142854&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume