

«beta»-terpinyl isobutyrate

Inchi:	InChI=1S/C14H24O2/c1-10(2)12-6-8-14(5,9-7-12)16-13(15)11(3)4/h11-12H,1,6-9H2,2-5H
InchiKey:	RKHBOAQGLKSIAH-UHFFFAOYSA-N
Formula:	C14H24O2
SMILES:	<chem>C=C(C)C1CCC(C)(OC(=O)C(C)C)CC1</chem>
Mol. weight [g/mol]:	224.34

Physical Properties

Property code	Value	Unit	Source
gf	-78.82	kJ/mol	Joback Method
hf	-417.51	kJ/mol	Joback Method
hfus	15.30	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.711		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1402.40		NIST Webbook
rinpol	1402.40		NIST Webbook
tb	607.25	K	Joback Method
tc	819.60	K	Joback Method
tf	316.02	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.01	J/mol×K	607.25	Joback Method
cpg	557.52	J/mol×K	642.64	Joback Method
cpg	576.91	J/mol×K	678.03	Joback Method
cpg	595.30	J/mol×K	713.43	Joback Method
cpg	612.79	J/mol×K	748.82	Joback Method
cpg	629.47	J/mol×K	784.21	Joback Method
cpg	645.46	J/mol×K	819.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R185098&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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