Isolinalyl acetate

Inchi: InChI=1S/C12H20O2/c1-6-12(5,14-11(4)13)9-7-8-10(2)3/h6H,1-2,7-9H2,3-5H3
InchiKey: RHPYMJUXEXERLP-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: C=CC(C)(CCCC(=C)C)OC(C)=O
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
hfus	18.34	kJ/mol	Joback Method
logp	3.241		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
rinpol	1238.00		NIST Webbook
rinpol	1238.00		NIST Webbook
tb	485.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.58	J/mol×K	540.26	Joback Method
cpg	443.36	J/mol×K	571.68	Joback Method
cpg	458.31	J/mol×K	603.11	Joback Method
cpg	472.48	J/mol×K	634.53	Joback Method
cpg	485.89	J/mol×K	665.96	Joback Method
cpg	498.57	J/mol×K	697.38	Joback Method
cpg	510.56	J/mol×K	728.81	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R284125&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature