Isolinalyl acetate

Inchi: InChI=1S/C12H20O2/c1-9(2)7-6-8-12(10(3)4)14-11(5)13/h7,12H,3,6,8H2,1-2,4-5H3
InchiKey: NRKPLVRYTKSVNC-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: C=C(C)C(CCC=C(C)C)OC(C)=O
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
hfus	22.40	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	492.68	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.81	J/mol×K	550.41	Joback Method
cpg	441.39	J/mol×K	581.95	Joback Method
cpg	456.21	J/mol×K	613.48	Joback Method
cpg	470.31	J/mol×K	645.02	Joback Method
cpg	483.71	J/mol×K	676.55	Joback Method
cpg	496.44	J/mol×K	708.09	Joback Method
cpg	508.52	J/mol×K	739.62	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R601882&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