neo-isopulegol acetate

Inchi: InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h9,11-12H,1,5-7H2,2-4H3/t9
InchiKey: HLHIVJRLODSUCI-USWWRNFRSA-N
Formula: C12H20O2
SMILES: C=C(C)C1CCC(C)CC1OC(C)=O
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-95.44	kJ/mol	Joback Method
hf	-406.53	kJ/mol	Joback Method
hfus	21.01	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.930		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1279.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1297.00		NIST Webbook
tb	557.02	K	Joback Method
tc	763.76	K	Joback Method
tf	280.34	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.53	J/mol×K	557.02	Joback Method
cpg	455.28	J/mol×K	591.48	Joback Method
cpg	474.03	J/mol×K	625.93	Joback Method
cpg	491.78	J/mol×K	660.39	Joback Method
cpg	508.54	J/mol×K	694.85	Joback Method

cpg	524.33	J/mol×K	729.31	Joback Method
cpg	539.15	J/mol×K	763.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235975&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume