Neopulegyl acetate

Inchi: InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h9,12H,5-7H2,1-4H3
InchiKey: ZAPTZQHAWAYFSW-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC(=O)OC1CC(C)CCC1=C(C)C
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-130.11	kJ/mol	Joback Method
hf	-435.59	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	52.45	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.075		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1263.00		NIST Webbook
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tb	571.65	K	Joback Method
tc	780.75	K	Joback Method
tf	296.70	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.34	J/mol×K	571.65	Joback Method
cpg	455.18	J/mol×K	606.50	Joback Method
cpg	473.04	J/mol×K	641.35	Joback Method
cpg	489.95	J/mol×K	676.20	Joback Method
cpg	505.91	J/mol×K	711.05	Joback Method
cpg	520.93	J/mol×K	745.90	Joback Method
cpg	535.03	J/mol×K	780.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R130117&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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