Norodovanone

Inchi: InChI=1S/C11H18O2/c1-5-11(4)7-6-10(13-11)8(2)9(3)12/h5,8,10H,1,6-7H2,2-4H3/t8-,10-
InchiKey: RNEVZQGFNUZDJC-JMJZKYOTSA-N
Formula: C11H18O2
SMILES: C=CC1(C)CCC(C(C)C(C)=O)O1
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-64.55	kJ/mol	Joback Method
hf	-339.42	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	49.08	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.335		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook
tb	538.99	K	Joback Method
tc	751.38	K	Joback Method
tf	304.03	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.77	J/mol×K	538.99	Joback Method
cpg	407.24	J/mol×K	574.39	Joback Method
cpg	423.61	J/mol×K	609.79	Joback Method
cpg	439.01	J/mol×K	645.19	Joback Method
cpg	453.55	J/mol×K	680.59	Joback Method
cpg	467.34	J/mol×K	715.99	Joback Method
cpg	480.50	J/mol×K	751.38	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=R516873&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