

Nordavanone

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
InchiKey: RNEVZQGFNUZDJC-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: C=CC1(C)CCC(C(C)C(C)=O)O1
Mol. weight [g/mol]: 182.26
CAS: 54933-91-4

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	1231.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1232.30		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1232.30		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	538.99	K	Joback Method
tc	751.38	K	Joback Method
tf	304.03	K	Joback Method
vc	0.592	m ³ /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:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C54933914&Units=SI

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

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