

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/t8?,10
InchiKey:	RNEVZQGFNUZDJC-GUJYYOPSSA-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
hfus	17.73	kJ/mol	Joback Method
logp	2.335		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
rinpol	1234.00		NIST Webbook

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R607395&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>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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