

Neointermedeol

Inchi:	InChI=1S/C15H26O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h12-13,16H,1,5-10H
InchiKey:	DPQYOKVMVCQHMY-ZQDZILKHS-A-N
Formula:	C15H26O
SMILES:	C=C(C)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
hfus	13.52	kJ/mol	Joback Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1660.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1660.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.33	J/mol×K	653.04	Joback Method
cpg	613.82	J/mol×K	688.52	Joback Method
cpg	633.38	J/mol×K	724.00	Joback Method
cpg	652.21	J/mol×K	759.48	Joback Method
cpg	670.53	J/mol×K	794.96	Joback Method
cpg	688.57	J/mol×K	830.44	Joback Method
cpg	706.54	J/mol×K	865.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R610712&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

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

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