

Intermedeol

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-GBJTYRQASA-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	1666.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1626.00		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		688.52	Joback Method
cpg	633.38		724.00	Joback Method
cpg	652.21		759.48	Joback Method
cpg	670.53		794.96	Joback Method
cpg	688.57		830.44	Joback Method
cpg	706.54		865.92	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R609113&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>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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