

cis-Muurool-5-en-4-«beta»-ol

Inchi: InChI=1S/C15H26O/c1-10(2)15(16)8-7-12(4)13-6-5-11(3)9-14(13)15/h9-13,16H,5-8H2,1
InchiKey: UAJHVFUBIKCODA-HNQLUHSGSA-N
Formula: C15H26O
SMILES: CC1C=C2C(CC1)C(C)CCC2(O)C(C)C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	19.72	kJ/mol	Joback Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1515.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.80	J/mol×K	659.94	Joback Method
cpg	617.79	J/mol×K	694.13	Joback Method
cpg	636.77	J/mol×K	728.33	Joback Method
cpg	654.86	J/mol×K	762.52	Joback Method
cpg	672.18	J/mol×K	796.72	Joback Method
cpg	688.83	J/mol×K	830.91	Joback Method
cpg	704.93	J/mol×K	865.11	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=R199903&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
rinpola:	Non-polar retention indices

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