

5-epi-Neointermedeol

Inchi:	InChI=1S/C15H28O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h11-13,16H,5-10H2
InchiKey:	PWTWAHBPEXYEQQ-MLGYPOCJSA-N
Formula:	C15H28O
SMILES:	CC(C)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]:	224.38

Physical Properties

Property code	Value	Unit	Source
gf	-17.14	kJ/mol	Joback Method
hf	-399.68	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.000		Crippen Method
mcvol	206.360	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1639.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1639.00		NIST Webbook
ripol	2219.00		NIST Webbook
ripol	2245.00		NIST Webbook
tb	656.04	K	Joback Method
tc	865.65	K	Joback Method
tf	365.75	K	Joback Method
vc	0.764	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.08	J/molxK	656.04	Joback Method
cpg	638.19	J/molxK	690.98	Joback Method
cpg	658.35	J/molxK	725.91	Joback Method
cpg	677.78	J/molxK	760.85	Joback Method

cpg	696.66	J/mol×K	795.78	Joback Method
cpg	715.22	J/mol×K	830.72	Joback Method
cpg	733.64	J/mol×K	865.65	Joback Method

Sources

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=R239828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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