

4,11,11-trimethyl-8-methylenebicyclo[7.2.0]undecane-4,5-diol

Inchi:	InChI=1S/C15H26O2/c1-9-5-6-12-11(8-15(12,3)4)10(2)7-13(16)14(9)17/h9,11-14,16-17H
InchiKey:	HFOYINMYDLCTSU-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	C=C1CC(O)C(O)C(C)CCC2C1CC2(C)C
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-120.47	kJ/mol	Joback Method
hf	-524.47	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	80.80	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.747		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
ripol	2706.00		NIST Webbook
tb	742.51	K	Joback Method
tc	938.91	K	Joback Method
tf	419.35	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.29	J/molxK	742.51	Joback Method
cpg	693.42	J/molxK	775.24	Joback Method
cpg	710.76	J/molxK	807.98	Joback Method
cpg	727.40	J/molxK	840.71	Joback Method
cpg	743.41	J/molxK	873.44	Joback Method
cpg	758.88	J/molxK	906.18	Joback Method
cpg	773.89	J/molxK	938.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R298832&Units=SI

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

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