

Gymnomitr-3(15)-en-4«beta»-ol

Inchi:	InChI=1S/C15H24O/c1-10-11-8-13(2,9-12(10)16)15(4)7-5-6-14(11,15)3/h11-12,16H,1,5-
InchiKey:	DDWYCTLZQKRVC-KNXMPVSZSA-N
Formula:	C15H24O
SMILES:	C=C1C(O)CC2(C)CC1C1(C)CCCC21C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	117.84	kJ/mol	Joback Method
hf	-209.80	kJ/mol	Joback Method
hfus	10.99	kJ/mol	Joback Method
hvap	61.83	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.530		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinsol	1659.00		NIST Webbook
tb	654.08	K	Joback Method
tc	869.16	K	Joback Method
tf	443.31	K	Joback Method
vc	0.726	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.34	J/mol×K	654.08	Joback Method
cpg	588.87	J/mol×K	689.93	Joback Method
cpg	606.74	J/mol×K	725.77	Joback Method
cpg	624.31	J/mol×K	761.62	Joback Method
cpg	641.90	J/mol×K	797.47	Joback Method
cpg	659.86	J/mol×K	833.31	Joback Method
cpg	678.52	J/mol×K	869.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R429511&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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