(+)-3-Gymnomitren-15-ol

Inchi: InChI=1S/C15H24O/c1-13-8-5-11(10-16)12(9-13)14(2)6-4-7-15(13,14)3/h5,12,16H,4,6-1
InchiKey: BOBUWMAINZVWRJ-XQLPTFJDSA-N
Formula: C15H24O
SMILES: CC12CC=C(CO)C(C1)C1(C)CCCC21C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	92.80	kJ/mol	Joback Method
hf	-227.39	kJ/mol	Joback Method
hfus	11.91	kJ/mol	Joback Method
hvap	62.94	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.531		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
tb	663.73	K	Joback Method
tc	879.86	K	Joback Method
tf	447.15	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.91	J/mol×K	663.73	Joback Method
cpg	586.84	J/mol×K	699.75	Joback Method
cpg	604.22	J/mol×K	735.77	Joback Method
cpg	621.43	J/mol×K	771.80	Joback Method
cpg	638.80	J/mol×K	807.82	Joback Method
cpg	656.69	J/mol×K	843.84	Joback Method
cpg	675.47	J/mol×K	879.86	Joback Method

Sources

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=R561323&Units=SI
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume