(-)-Gymnomitr-3(15)-en-12-al

Inchi: InChI=1S/C15H22O/c1-11-5-8-13(2)9-12(11)15(10-16)7-4-6-14(13,15)3/h10,12H,1,4-9H2
InchiKey: WQOYFPJIOSPRJD-WLUIXCMPSA-N
Formula: C15H22O
SMILES: C=C1CCC2(C)CC1C1(C=O)CCCC21C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	162.85	kJ/mol	Joback Method
hf	-122.81	kJ/mol	Joback Method
hfus	8.12	kJ/mol	Joback Method
hvap	52.18	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1632.00		NIST Webbook
tb	615.23	K	Joback Method
tc	850.74	K	Joback Method
tf	428.73	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.98	J/mol×K	615.23	Joback Method
cpg	545.98	J/mol×K	654.48	Joback Method
cpg	564.83	J/mol×K	693.73	Joback Method
cpg	583.00	J/mol×K	732.99	Joback Method
cpg	600.94	J/mol×K	772.24	Joback Method
cpg	619.09	J/mol×K	811.49	Joback Method
cpg	637.91	J/mol×K	850.74	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=R561670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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