(+)-Gymnomitr-3(15)-en-12-oic acid

Inchi: InChI=1S/C15H22O2/c1-10-5-8-13(2)9-11(10)15(12(16)17)7-4-6-14(13,15)3/h11H,1,4-9H
InchiKey: VDQVZUARIGBYPI-KVPGNWIISA-N
Formula: C15H22O2
SMILES: C=C1CCC2(C)CC1C1(C(=O)O)CCCC21C
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-3.37	kJ/mol	Joback Method
hf	-302.04	kJ/mol	Joback Method
hfus	11.52	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.624		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	712.62	K	Joback Method
tc	933.88	K	Joback Method
tf	497.48	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.87	J/mol×K	712.62	Joback Method
cpg	606.11	J/mol×K	749.50	Joback Method
cpg	623.28	J/mol×K	786.37	Joback Method
cpg	640.75	J/mol×K	823.25	Joback Method
cpg	658.89	J/mol×K	860.13	Joback Method
cpg	678.08	J/mol×K	897.00	Joback Method
cpg	698.69	J/mol×K	933.88	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=R561487&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