(-)-Gymnomitr-3(15)-en-4-one

Inchi: InChI=1S/C15H22O/c1-10-11-8-13(2,9-12(10)16)15(4)7-5-6-14(11,15)3/h11H,1,5-9H2,2-
InchiKey: AQEVLQOUEXYZOS-WKOCEIDGSA-N
Formula: C15H22O
SMILES: C=C1C(=O)CC2(C)CC1C1(C)CCCC21C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	139.78	kJ/mol	Joback Method
hf	-174.93	kJ/mol	Joback Method
hfus	5.34	kJ/mol	Joback Method
hvap	49.71	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1633.00		NIST Webbook
tb	634.39	K	Joback Method
tc	881.30	K	Joback Method
tf	454.95	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.43	J/mol×K	634.39	Joback Method
cpg	558.75	J/mol×K	675.54	Joback Method
cpg	579.13	J/mol×K	716.69	Joback Method
cpg	599.03	J/mol×K	757.84	Joback Method
cpg	618.95	J/mol×K	799.00	Joback Method
cpg	639.33	J/mol×K	840.15	Joback Method
cpg	660.67	J/mol×K	881.30	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=R561685&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