10-Epigazaniolide

Inchi: InChI=1S/C15H18O2/c1-9-5-4-7-15(3)8-6-11-10(2)14(16)17-13(11)12(9)15/h4-5,7,11-13
InchiKey: MKOHVWLOSUZFFH-UHFFFAOYSA-N
Formula: C15H18O2
SMILES: C=C1C(=O)OC2C1CCC1(C)C=CC=C(C)C21
Mol. weight [g/mol]: 230.30
CAS: 193698-44-1

Physical Properties

Property code	Value	Unit	Source
gf	90.73	kJ/mol	Joback Method
hf	-245.64	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	58.11	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.017		Crippen Method
mcvol	184.170	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	1832.60		NIST Webbook
tb	672.70	K	Joback Method
tc	918.69	K	Joback Method
tf	440.72	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.05	J/mol×K	672.70	Joback Method
cpg	556.13	J/mol×K	713.70	Joback Method
cpg	575.07	J/mol×K	754.70	Joback Method
cpg	593.03	J/mol×K	795.69	Joback Method
cpg	610.22	J/mol×K	836.69	Joback Method
cpg	626.81	J/mol×K	877.69	Joback Method
cpg	643.00	J/mol×K	918.69	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=C193698441&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

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