Jalcaguaianolide

Inchi: InChI=1S/C15H18O2/c1-8-4-7-12-10(3)15(16)17-14(12)13-9(2)5-6-11(8)13/h5,11,13-14H
InchiKey: WAQFXLYLGJEYAW-AYBZEELNSA-N
Formula: C15H18O2
SMILES: C=C1CCC2=C(C)C(=O)OC2C2C(C)=CCC12
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	84.67	kJ/mol	Joback Method
hf	-263.48	kJ/mol	Joback Method
hfus	28.22	kJ/mol	Joback Method
hvap	60.90	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.161		Crippen Method
mcvol	184.170	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1939.00		NIST Webbook
tb	687.09	K	Joback Method
tc	925.52	K	Joback Method
tf	446.10	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.69	J/mol×K	687.09	Joback Method
cpg	555.78	J/mol×K	726.83	Joback Method
cpg	573.58	J/mol×K	766.57	Joback Method
cpg	590.13	J/mol×K	806.30	Joback Method
cpg	605.48	J/mol×K	846.04	Joback Method
cpg	619.68	J/mol×K	885.78	Joback Method
cpg	632.78	J/mol×K	925.52	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=R194899&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