Germacrol

Inchi: InChI=1S/C15H22O/c1-11(2)14-9-8-12(3)6-5-7-13(4)10-15(14)16/h7-8H,5-6,9-10H2,1-4H
InchiKey: CAULGCQHVOVVRN-UPAULDTKSA-N
Formula: C15H22O
SMILES: CC1=CCC(=C(C)C)C(=O)CC(C)=CCC1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	14.16	kJ/mol	Joback Method
hf	-281.75	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.359		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
tb	666.52	K	Joback Method
tc	907.31	K	Joback Method
tf	347.53	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.74	J/mol×K	666.52	Joback Method
cpg	561.51	J/mol×K	706.65	Joback Method
cpg	581.83	J/mol×K	746.78	Joback Method
cpg	600.67	J/mol×K	786.92	Joback Method
cpg	618.01	J/mol×K	827.05	Joback Method
cpg	633.82	J/mol×K	867.18	Joback Method
cpg	648.08	J/mol×K	907.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R324906&Units=SI

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