Geijerone

Inchi: InChI=1S/C11H16O/c1-4-9-5-6-10(12)7-11(9)8(2)3/h4,9,11H,1-2,5-7H2,3H3
InchiKey: GPJWYPULQMBLGX-UHFFFAOYSA-N
Formula: C11H16O
SMILES: C=CC1CCC(=O)CC1C(=C)C
Mol. weight [g/mol]: 164.24

Physical Properties

Property code	Value	Unit	Source
gf	103.02	kJ/mol	Joback Method
hf	-133.02	kJ/mol	Joback Method
hfus	12.79	kJ/mol	Joback Method
hvap	43.19	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.734		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
tb	527.02	K	Joback Method
tc	750.43	K	Joback Method
tf	267.61	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.60	J/mol×K	527.02	Joback Method
cpg	367.85	J/mol×K	564.25	Joback Method
cpg	386.09	J/mol×K	601.49	Joback Method
cpg	403.33	J/mol×K	638.72	Joback Method
cpg	419.59	J/mol×K	675.96	Joback Method
cpg	434.86	J/mol×K	713.19	Joback Method
cpg	449.16	J/mol×K	750.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R83998&Units=SI
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

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