(Z)-«alpha»-Damascenone

Inchi: InChI=1S/C13H18O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5-9,12H,1-4H3/b7-5-
InchiKey: JGBBQKAJVHEQJM-ALCCZGGFSA-N
Formula: C13H18O
SMILES: CC=CC(=O)C1C(C)=CC=CC1(C)C
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
gf	71.42	kJ/mol	Joback Method
hf	-153.70	kJ/mol	Joback Method
hfus	19.89	kJ/mol	Joback Method
hvap	51.45	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.290		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1352.00		NIST Webbook
tb	573.29	K	Joback Method
tc	793.42	K	Joback Method
tf	322.20	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.67	J/mol×K	573.29	Joback Method
cpg	436.18	J/mol×K	609.98	Joback Method
cpg	452.61	J/mol×K	646.67	Joback Method
cpg	468.10	J/mol×K	683.35	Joback Method
cpg	482.77	J/mol×K	720.04	Joback Method
cpg	496.77	J/mol×K	756.73	Joback Method
cpg	510.21	J/mol×K	793.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R517792&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