Damascenone A

Inchi: InChI=1S/C13H18O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5-8H,9H2,1-4H3/b7-5-
InchiKey: POIARNZEYGURDG-ALCCZGGFSA-N
Formula: C13H18O
SMILES: CC=CC(=O)C1=C(C)C=CCC1(C)C
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
gf	69.50	kJ/mol	Joback Method
hf	-144.83	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.434		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1476.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1891.00		NIST Webbook
tb	582.94	K	Joback Method
tc	804.13	K	Joback Method
tf	338.96	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.12	J/mol×K	582.94	Joback Method
cpg	433.84	J/mol×K	619.80	Joback Method
cpg	449.57	J/mol×K	656.67	Joback Method
cpg	464.42	J/mol×K	693.53	Joback Method
cpg	478.54	J/mol×K	730.40	Joback Method
cpg	492.06	J/mol×K	767.26	Joback Method
cpg	505.11	J/mol×K	804.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341738&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume