3-oxo-R-damascone 1

Inchi: InChI=1S/C13H18O2/c1-5-6-11(15)12-9(2)7-10(14)8-13(12,3)4/h5-6H,7-8H2,1-4H3/b6-5
InchiKey: IVBOBZYOBZBYMI-AATRIKPKSA-N
Formula: C13H18O2
SMILES: CC=CC(=O)C1=C(C)CC(=O)CC1(C)C
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-83.05	kJ/mol	Joback Method
hf	-340.31	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Joback Method
hvap	56.38	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.837		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
ripol	2438.00		NIST Webbook
ripol	2438.00		NIST Webbook
tb	651.60	K	Joback Method
tc	883.18	K	Joback Method
tf	406.42	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.71	J/mol×K	651.60	Joback Method
cpg	485.89	J/mol×K	690.20	Joback Method
cpg	502.22	J/mol×K	728.79	Joback Method
cpg	517.81	J/mol×K	767.39	Joback Method
cpg	532.78	J/mol×K	805.99	Joback Method
cpg	547.23	J/mol×K	844.58	Joback Method
cpg	561.29	J/mol×K	883.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R332977&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume