4-hydroxy-«beta»-damascone

Inchi: InChI=1S/C12H18O2/c1-4-5-11(14)10-7-6-9(13)8-12(10,2)3/h4-5,7,9,13H,6,8H2,1-3H3/b
InchiKey: ZFOVDQCWKGLFBS-SNAWJCMRSA-N
Formula: C12H18O2
SMILES: CC=CC(=O)C1=CCC(O)CC1(C)C
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-103.78	kJ/mol	Joback Method
hf	-343.07	kJ/mol	Joback Method
hfus	20.17	kJ/mol	Joback Method
hvap	65.61	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.239		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
ripol	2451.00		NIST Webbook
tb	643.43	K	Joback Method
tc	849.34	K	Joback Method
tf	370.99	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.38	J/mol×K	643.43	Joback Method
cpg	464.03	J/mol×K	677.75	Joback Method
cpg	477.94	J/mol×K	712.07	Joback Method
cpg	491.22	J/mol×K	746.39	Joback Method
cpg	503.98	J/mol×K	780.70	Joback Method
cpg	516.33	J/mol×K	815.02	Joback Method
cpg	528.37	J/mol×K	849.34	Joback Method

Sources

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=R389196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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