Isomethyl-«alpha»-damascone

Inchi: InChI=1S/C14H22O/c1-6-10(2)13(15)12-11(3)8-7-9-14(12,4)5/h6H,7-9H2,1-5H3/b10-6+
InchiKey: HFNLNVUEMZKZCC-UXBLZVDNSA-N
Formula: C14H22O
SMILES: CC=C(C)C(=O)C1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	39.41	kJ/mol	Joback Method
hf	-233.04	kJ/mol	Joback Method
hfus	18.49	kJ/mol	Joback Method
hvap	54.44	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.048		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	606.54	K	Joback Method
tc	825.60	K	Joback Method
tf	335.51	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.69	J/mol×K	606.54	Joback Method
cpg	506.36	J/mol×K	643.05	Joback Method
cpg	523.99	J/mol×K	679.56	Joback Method
cpg	540.71	J/mol×K	716.07	Joback Method
cpg	556.67	J/mol×K	752.58	Joback Method
cpg	571.99	J/mol×K	789.09	Joback Method
cpg	586.80	J/mol×K	825.60	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=R325865&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume