(Z)-«alpha»-Damascone

Other names: cis-«alpha»-Damascone
«alpha»-Z-damascone
Inchi: InChI=1S/C13H20O/c1-5-6-12(14)11-9-10(2)7-8-13(11,3)4/h5-6,9,11H,7-8H2,1-4H3/b6-5
InchiKey: XJPSXUXZJUPQNM-WAYWQWQTSA-N
Formula: C13H20O
SMILES: CC=CC(=O)C1C=C(C)CCC1(C)C
Mol. weight [g/mol]: 192.30
CAS: 57549-93-6

Physical Properties

Property code	Value	Unit	Source
gf	41.46	kJ/mol	Joback Method
hf	-211.48	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	51.16	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.514		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1366.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	574.13	K	Joback Method
tc	792.17	K	Joback Method
tf	321.44	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	438.46	J/mol×K	574.13	Joback Method
cpg	457.12	J/mol×K	610.47	Joback Method
cpg	474.66	J/mol×K	646.81	Joback Method
cpg	491.22	J/mol×K	683.15	Joback Method
cpg	506.92	J/mol×K	719.49	Joback Method
cpg	521.90	J/mol×K	755.83	Joback Method
cpg	536.27	J/mol×K	792.17	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=C57549936&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