«alpha»-Damascone

Inchi:	InChI=1S/C13H20O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5,8,12H,1,6-7,9H2,2-4H3
InchiKey:	GCGZDUFEEQNVPR-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	C=CCC(=O)C1C(C)=CCCC1(C)C
Mol. weight [g/mol]:	192.30
CAS:	31089-90-4

Physical Properties

Property code	Value	Unit	Source
gf	49.08	kJ/mol	Joback Method
hf	-203.27	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	50.53	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.514		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	1384.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1386.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1812.00		NIST Webbook
tb	566.65	K	Joback Method
tc	779.77	K	Joback Method
tf	324.76	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.08	J/mol×K	566.65	Joback Method
cpg	455.58	J/mol×K	602.17	Joback Method

cpg	473.01	J/mol×K	637.69	Joback Method
cpg	489.48	J/mol×K	673.21	Joback Method
cpg	505.09	J/mol×K	708.73	Joback Method
cpg	519.97	J/mol×K	744.25	Joback Method
cpg	534.22	J/mol×K	779.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31089904&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

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