3-Hydroxy-«beta»-damascone

Inchi: InChI=1S/C13H20O2/c1-5-6-11(15)12-9(2)10(14)7-8-13(12,3)4/h5-6,10,14H,7-8H2,1-4H
InchiKey: NOORESDHJXLGAO-AATRIKPKSA-N
Formula: C13H20O2
SMILES: CC=CC(=O)C1=C(C)C(O)CCC1(C)C
Mol. weight [g/mol]: 208.30
CAS: 102488-09-5

Physical Properties

Property code	Value	Unit	Source
gf	-104.99	kJ/mol	Joback Method
hf	-375.18	kJ/mol	Joback Method
hfus	22.37	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1627.00		NIST Webbook
ripol	2535.00		NIST Webbook
ripol	2532.00		NIST Webbook
ripol	2559.00		NIST Webbook
ripol	2537.00		NIST Webbook
ripol	2537.00		NIST Webbook
ripol	2535.00		NIST Webbook
ripol	2546.00		NIST Webbook
ripol	2559.00		NIST Webbook
ripol	2544.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2537.00		NIST Webbook

ripol	2537.00		NIST Webbook
ripol	2525.00		NIST Webbook
ripol	2531.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2504.00		NIST Webbook
ripol	2504.00		NIST Webbook
ripol	2537.00		NIST Webbook
ripol	2532.00		NIST Webbook
ripol	2535.00		NIST Webbook
tb	671.29	K	Joback Method
tc	875.23	K	Joback Method
tf	394.78	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.33	J/mol×K	671.29	Joback Method
cpg	515.41	J/mol×K	705.28	Joback Method
cpg	529.82	J/mol×K	739.27	Joback Method
cpg	543.66	J/mol×K	773.26	Joback Method
cpg	557.02	J/mol×K	807.25	Joback Method
cpg	570.02	J/mol×K	841.24	Joback Method
cpg	582.75	J/mol×K	875.23	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=C102488095&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume