

(Z)-«beta»-Damascone

Other names:	«beta»-(Z)-damascone
Inchi:	InChI=1S/C13H20O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5,7,12H,2,6,8-9H2,1,3-4H3/
InchiKey:	IXLLBXDECOMIBP-ALCCZGGFSA-N
Formula:	C13H20O
SMILES:	<chem>C=C1CCCC(C)(C)C1C(=O)C=CC</chem>
Mol. weight [g/mol]:	192.30

Physical Properties

Property code	Value	Unit	Source
gf	74.21	kJ/mol	Joback Method
hf	-173.55	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.514		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	1383.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1383.00		NIST Webbook
tb	569.15	K	Joback Method
tc	785.96	K	Joback Method
tf	321.84	K	Joback Method
vc	0.663	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.42	J/mol×K	569.15	Joback Method

cpg	456.28	J/mol×K	605.28	Joback Method
cpg	474.02	J/mol×K	641.42	Joback Method
cpg	490.76	J/mol×K	677.55	Joback Method
cpg	506.62	J/mol×K	713.69	Joback Method
cpg	521.73	J/mol×K	749.82	Joback Method
cpg	536.20	J/mol×K	785.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R302253&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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