2-Cyclopenten-1-one, 2-(2-butenyl)-4-hydroxy-3-methyl-, (Z)-

Other names: Cinerolon
Cinerolone
2-[(2Z)-2-Butenyl]-4-hydroxy-3-methyl-2-cyclopenten-1-one
cis -Cinerolone
Z-Cinerolone

Inchi: InChI=1S/C10H14O2/c1-3-4-5-8-7(2)9(11)6-10(8)12/h3-4,9,11H,5-6H2,1-2H3/b4-3-

InchiKey: YLKLJBPHNWWPSF-ARJAWSKDSA-N

Formula: C10H14O2

SMILES: CC=CCC1=C(C)C(O)CC1=O

Mol. weight [g/mol]: 166.22

CAS: 17190-74-8

Physical Properties

Property code	Value	Unit	Source
gf	-98.62	kJ/mol	Joback Method
hf	-327.12	kJ/mol	Joback Method
hfus	19.84	kJ/mol	Joback Method
hvap	60.61	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.603		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	1641.00		NIST Webbook
tb	616.76	K	Joback Method
tc	821.12	K	Joback Method
tf	363.12	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.96	J/mol×K	616.76	Joback Method
cpg	370.95	J/mol×K	650.82	Joback Method
cpg	383.28	J/mol×K	684.88	Joback Method

cpg	394.98	J/mol×K	718.94	Joback Method
cpg	406.04	J/mol×K	753.00	Joback Method
cpg	416.48	J/mol×K	787.06	Joback Method
cpg	426.31	J/mol×K	821.12	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=C17190748&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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