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

Other names: (Z)-Cinerone
Cineron
Cinerone

Inchi: InChI=1S/C10H14O/c1-3-4-5-9-8(2)6-7-10(9)11/h3-4H,5-7H2,1-2H3/b4-3-

InchiKey: IVLCENBZDYVJPA-ARJAWSKDSA-N

Formula: C10H14O

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

Mol. weight [g/mol]: 150.22

CAS: 17190-71-5

Physical Properties

Property code	Value	Unit	Source
gf	45.91	kJ/mol	Joback Method
hf	-154.55	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	44.24	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.632		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1183.80		NIST Webbook
rinpol	1183.80		NIST Webbook
tb	529.25	K	Joback Method
tc	749.45	K	Joback Method
tf	306.54	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.05	J/mol×K	529.25	Joback Method
cpg	317.21	J/mol×K	565.95	Joback Method
cpg	331.59	J/mol×K	602.65	Joback Method
cpg	345.21	J/mol×K	639.35	Joback Method

cpg	358.11	J/mol×K	676.05	Joback Method
cpg	370.28	J/mol×K	712.75	Joback Method
cpg	381.77	J/mol×K	749.45	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=C17190715&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