

«alpha»-Methyl crotonolactone

Inchi:	InChI=1S/C5H8O2/c1-3-4(2)7-5(3)6/h3-4H,1-2H3
InchiKey:	IABBAPSDOJPBAF-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC1OC(=O)C1C
Mol. weight [g/mol]:	100.12

Physical Properties

Property code	Value	Unit	Source
gf	-176.55	kJ/mol	Joback Method
hf	-369.93	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	35.26	kJ/mol	Joback Method
log10ws	-0.54		Crippen Method
logp	0.568		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
ripol	1687.00		NIST Webbook
ripol	1687.00		NIST Webbook
tb	414.91	K	Joback Method
tc	625.45	K	Joback Method
tf	251.08	K	Joback Method
vc	0.291	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.89	J/mol×K	414.91	Joback Method
cpg	167.78	J/mol×K	450.00	Joback Method
cpg	178.29	J/mol×K	485.09	Joback Method
cpg	188.42	J/mol×K	520.18	Joback Method
cpg	198.16	J/mol×K	555.27	Joback Method
cpg	207.49	J/mol×K	590.36	Joback Method
cpg	216.42	J/mol×K	625.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R345156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
ripl:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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