

Cyclopropanecarboxylic acid, 3-methylbut-2-enyl ester

Inchi:	InChI=1S/C9H14O2/c1-7(2)5-6-11-9(10)8-3-4-8/h5,8H,3-4,6H2,1-2H3
InchiKey:	QKSQPNPCCOABAK-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CC(C)=CCOC(=O)C1CC1
Mol. weight [g/mol]:	154.21

Physical Properties

Property code	Value	Unit	Source
gf	-76.60	kJ/mol	Joback Method
hf	-293.66	kJ/mol	Joback Method
hfus	18.88	kJ/mol	Joback Method
hvap	44.73	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.906		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
tb	492.39	K	Joback Method
tc	691.60	K	Joback Method
tf	262.25	K	Joback Method
vc	0.501	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.34	J/mol×K	492.39	Joback Method
cpg	305.44	J/mol×K	525.59	Joback Method
cpg	318.76	J/mol×K	558.79	Joback Method
cpg	331.33	J/mol×K	591.99	Joback Method
cpg	343.19	J/mol×K	625.20	Joback Method
cpg	354.38	J/mol×K	658.40	Joback Method
cpg	364.94	J/mol×K	691.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299374&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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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