

Cyclobutanecarboxylic acid, 3-methylbut-2-enyl ester

Inchi:	InChI=1S/C10H16O2/c1-8(2)6-7-12-10(11)9-4-3-5-9/h6,9H,3-5,7H2,1-2H3
InchiKey:	WAELPPWICIWJKF-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CC(C)=CCOC(=O)C1CCC1
Mol. weight [g/mol]:	168.23

Physical Properties

Property code	Value	Unit	Source
gf	-80.28	kJ/mol	Joback Method
hf	-320.46	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	47.13	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.296		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1218.00		NIST Webbook
tb	519.54	K	Joback Method
tc	723.26	K	Joback Method
tf	270.00	K	Joback Method
vc	0.549	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.59	J/mol×K	519.54	Joback Method
cpg	352.42	J/mol×K	553.49	Joback Method
cpg	367.38	J/mol×K	587.45	Joback Method
cpg	381.50	J/mol×K	621.40	Joback Method
cpg	394.81	J/mol×K	655.35	Joback Method
cpg	407.37	J/mol×K	689.30	Joback Method
cpg	419.20	J/mol×K	723.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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