

Cyclobutanecarboxylic acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C8H11ClO2/c9-5-2-6-11-8(10)7-3-1-4-7/h2,5,7H,1,3-4,6H2/b5-2+
InchiKey:	PWMURWCEFOHIHN-GORDUTHDSA-N
Formula:	C8H11ClO2
SMILES:	O=C(OCC=CCl)C1CCC1
Mol. weight [g/mol]:	174.62

Physical Properties

Property code	Value	Unit	Source
gf	-100.50	kJ/mol	Joback Method
hf	-285.13	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	46.99	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.082		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinqol	1208.00		NIST Webbook
tb	511.33	K	Joback Method
tc	722.52	K	Joback Method
tf	291.34	K	Joback Method
vc	0.485	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.87	J/molxK	511.33	Joback Method
cpg	332.64	J/molxK	687.32	Joback Method
cpg	322.52	J/molxK	652.12	Joback Method
cpg	311.72	J/molxK	616.92	Joback Method
cpg	300.21	J/molxK	581.73	Joback Method
cpg	287.94	J/molxK	546.53	Joback Method
cpg	342.11	J/molxK	722.52	Joback Method
dvisc	0.0003642	Paxs	511.33	Joback Method
dvisc	0.0004417	Paxs	474.66	Joback Method

dvisc	0.0005533	Paxs	438.00	Joback Method
dvisc	0.0007222	Paxs	401.34	Joback Method
dvisc	0.0009945	Paxs	364.67	Joback Method
dvisc	0.0014710	Paxs	328.00	Joback Method
dvisc	0.0024011	Paxs	291.34	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=U299138&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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