

Cis-3-chlorocrotonic acid

Inchi:	InChI=1S/C4H5ClO2/c1-3(5)2-4(6)7/h1-2H2,(H,6,7)
InchiKey:	OSNGODILMZETAU-UHFFFAOYSA-N
Formula:	C4H5ClO2
SMILES:	C=C(Cl)CC(=O)O
Mol. weight [g/mol]:	120.53

Physical Properties

Property code	Value	Unit	Source
gf	-215.58	kJ/mol	Joback Method
hf	-290.80	kJ/mol	Joback Method
hfus	13.41	kJ/mol	Joback Method
hvap	51.72	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.214		Crippen Method
mvol	82.600	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
tb	470.96	K	Joback Method
tc	658.06	K	Joback Method
tf	259.79	K	Joback Method
vc	0.316	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.56	J/mol×K	470.96	Joback Method
cpg	156.13	J/mol×K	502.14	Joback Method
cpg	161.40	J/mol×K	533.33	Joback Method
cpg	166.39	J/mol×K	564.51	Joback Method
cpg	171.10	J/mol×K	595.69	Joback Method
cpg	175.56	J/mol×K	626.87	Joback Method
cpg	179.76	J/mol×K	658.06	Joback Method

Sources

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=B6000274&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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