

cis-3-Chloro-2-butenic acid

Inchi:	InChI=1S/C4H5ClO2/c1-3(5)2-4(6)7/h2H,1H3,(H,6,7)/b3-2-
InchiKey:	XBOTUWGQYMHUFO-IHWYPQMZSA-N
Formula:	C4H5ClO2
SMILES:	CC(Cl)=CC(=O)O
Mol. weight [g/mol]:	120.53
CAS:	55831-56-6

Physical Properties

Property code	Value	Unit	Source
gf	-223.20	kJ/mol	Joback Method
hf	-299.01	kJ/mol	Joback Method
hfus	14.89	kJ/mol	Joback Method
hvap	52.35	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.214		Crippen Method
mcvol	82.600	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
tb	478.44	K	Joback Method
tc	670.43	K	Joback Method
tf	256.47	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.48	J/molxK	638.43	Joback Method
cpg	149.23	J/molxK	478.44	Joback Method
cpg	154.92	J/molxK	510.44	Joback Method
cpg	160.27	J/molxK	542.44	Joback Method
cpg	165.31	J/molxK	574.43	Joback Method
cpg	170.04	J/molxK	606.43	Joback Method
cpg	178.67	J/molxK	670.43	Joback Method
cps	140.20	J/molxK	298.00	NIST Webbook
hfust	13.81	kJ/mol	333.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55831566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

cp_g:	Ideal gas heat capacity
cp_s:	Solid phase heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{fust}:	Enthalpy of fusion at a given temperature
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
sf_{ust}:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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