

3-(2-Chlorophenyl)propionic acid

Inchi:	InChI=1S/C9H9ClO2/c10-8-4-2-1-3-7(8)5-6-9(11)12/h1-4H,5-6H2,(H,11,12)
InchiKey:	KZMDFTFGWIVSNQ-UHFFFAOYSA-N
Formula:	C9H9ClO2
SMILES:	O=C(O)CCc1ccccc1Cl
Mol. weight [g/mol]:	184.62
CAS:	1643-28-3

Physical Properties

Property code	Value	Unit	Source
gf	-149.99	kJ/mol	Joback Method
hf	-284.58	kJ/mol	Joback Method
hfus	22.60	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.357		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	620.46	K	Joback Method
tc	828.56	K	Joback Method
tf	370.80	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.06	J/mol×K	620.46	Joback Method
cpg	344.67	J/mol×K	793.88	Joback Method
cpg	337.46	J/mol×K	759.19	Joback Method
cpg	329.72	J/mol×K	724.51	Joback Method
cpg	321.43	J/mol×K	689.83	Joback Method
cpg	312.55	J/mol×K	655.14	Joback Method
cpg	351.37	J/mol×K	828.56	Joback Method
dvisc	0.0000910	Pa×s	620.46	Joback Method
dvisc	0.0001330	Pa×s	578.85	Joback Method

dvisc	0.0002062	Pa×s	537.24	Joback Method
dvisc	0.0003441	Pa×s	495.63	Joback Method
dvisc	0.0006307	Pa×s	454.02	Joback Method
dvisc	0.0013065	Pa×s	412.41	Joback Method
dvisc	0.0031870	Pa×s	370.80	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=C1643283&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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