

3-(3,4-Dichlorophenyl)propionic acid

Inchi:	InChI=1S/C9H8Cl2O2/c10-7-3-1-6(5-8(7)11)2-4-9(12)13/h1,3,5H,2,4H2,(H,12,13)
InchiKey:	NHYJRLYFKZYPMO-UHFFFAOYSA-N
Formula:	C9H8Cl2O2
SMILES:	O=C(O)CCc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	219.06
CAS:	25173-68-6

Physical Properties

Property code	Value	Unit	Source
gf	-171.55	kJ/mol	Joback Method
hf	-311.79	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	71.42	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.011		Crippen Method
mcvol	145.830	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	662.87	K	Joback Method
tc	875.40	K	Joback Method
tf	413.24	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.70	J/molxK	662.87	Joback Method
cpg	359.88	J/molxK	839.98	Joback Method
cpg	353.49	J/molxK	804.56	Joback Method
cpg	346.59	J/molxK	769.13	Joback Method
cpg	339.18	J/molxK	733.71	Joback Method
cpg	331.22	J/molxK	698.29	Joback Method
cpg	365.81	J/molxK	875.40	Joback Method
dvisc	0.0000756	Paxs	662.87	Joback Method
dvisc	0.0001065	Paxs	621.26	Joback Method

dvisc	0.0001577	Paxs	579.66	Joback Method
dvisc	0.0002481	Paxs	538.06	Joback Method
dvisc	0.0004211	Paxs	496.45	Joback Method
dvisc	0.0007875	Paxs	454.85	Joback Method
dvisc	0.0016703	Paxs	413.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25173686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
mccvol:	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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