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/mol×K	662.87	Joback Method
cpg	331.22	J/mol×K	698.29	Joback Method
cpg	339.18	J/mol×K	733.71	Joback Method
cpg	346.59	J/mol×K	769.13	Joback Method
cpg	353.49	J/mol×K	804.56	Joback Method
cpg	359.88	J/mol×K	839.98	Joback Method
cpg	365.81	J/mol×K	875.40	Joback Method
dvisc	0.0016703	Pa×s	413.24	Joback Method
dvisc	0.0007875	Pa×s	454.85	Joback Method

dvisc	0.0004211	Pa×s	496.45	Joback Method
dvisc	0.0002481	Pa×s	538.06	Joback Method
dvisc	0.0001577	Pa×s	579.66	Joback Method
dvisc	0.0001065	Pa×s	621.26	Joback Method
dvisc	0.0000756	Pa×s	662.87	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=C25173686&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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