

3,4-Dichlorophenylacetic acid

Other names:	Benzeneacetic acid, 3,4-dichloro-
Inchi:	InChI=1S/C8H6Cl2O2/c9-6-2-1-5(3-7(6)10)4-8(11)12/h1-3H,4H2,(H,11,12)
InchiKey:	ZOUPGSMNQLUNW-UHFFFAOYSA-N
Formula:	C8H6Cl2O2
SMILES:	O=C(O)Cc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	205.04
CAS:	5807-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-179.97	kJ/mol	Joback Method
hf	-291.15	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.620		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	639.99	K	Joback Method
tc	856.02	K	Joback Method
tf	401.97	K	Joback Method
vc	0.498	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.15	J/molxK	639.99	Joback Method
cpg	309.36	J/molxK	820.01	Joback Method
cpg	303.68	J/molxK	784.01	Joback Method
cpg	297.54	J/molxK	748.00	Joback Method
cpg	290.92	J/molxK	712.00	Joback Method
cpg	283.80	J/molxK	675.99	Joback Method
cpg	314.61	J/molxK	856.02	Joback Method
dvisc	0.0000895	Paxs	639.99	Joback Method

dvisc	0.0001258	Paxs	600.32	Joback Method
dvisc	0.0001857	Paxs	560.65	Joback Method
dvisc	0.0002908	Paxs	520.98	Joback Method
dvisc	0.0004904	Paxs	481.31	Joback Method
dvisc	0.0009085	Paxs	441.64	Joback Method
dvisc	0.0019005	Paxs	401.97	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5807307&Units=SI

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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