

2,2-Bis(4-chlorophenyl)acetic acid

Other names:	Benzeneacetic acid, 4-chloro-«alpha»-(4-chlorophenyl)- Acetic acid, bis(p-chlorophenyl)- p,p'-DDA Bis(p-chlorophenyl)acetic acid Bis(4-chlorophenyl)acetic acid Di(p-chlorophenyl)acetic acid Dichlorodiphenylacetic acid DDA DDA, (Degradation product) p,p'-Dichlorodiphenylacetic acid Bis(p-chlorophenyl)essigsaeure 2,2-Bis(p-chlorophenyl)acetic acid Acetic acid, bis-(4-chlorophenyl) NSC 4279
Inchi:	InChI=1S/C14H10Cl2O2/c15-11-5-1-9(2-6-11)13(14(17)18)10-3-7-12(16)8-4-10/h1-8,13H
InchiKey:	YIOCIFXUGBYCJR-UHFFFAOYSA-N
Formula:	C14H10Cl2O2
SMILES:	O=C(O)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	281.13
CAS:	83-05-6

Physical Properties

Property code	Value	Unit	Source
gf	-19.48	kJ/mol	Joback Method
hf	-183.74	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	84.44	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.210		Crippen Method
mcvol	192.520	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpola	1933.00		NIST Webbook
tb	803.51	K	Joback Method
tc	1039.98	K	Joback Method
tf	441.26 ± 0.20	K	NIST Webbook
vc	0.721	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.47	J/molxK	1039.98	Joback Method
cpg	523.33	J/molxK	1000.57	Joback Method
cpg	516.58	J/molxK	961.16	Joback Method
cpg	509.16	J/molxK	921.74	Joback Method
cpg	500.99	J/molxK	882.33	Joback Method
cpg	492.02	J/molxK	842.92	Joback Method
cpg	482.18	J/molxK	803.51	Joback Method
dvisc	0.0007544	Paxs	481.01	Joback Method
dvisc	0.0000282	Paxs	803.51	Joback Method
dvisc	0.0000401	Paxs	749.76	Joback Method
dvisc	0.0000601	Paxs	696.01	Joback Method
dvisc	0.0000965	Paxs	642.26	Joback Method
dvisc	0.0001690	Paxs	588.51	Joback Method
dvisc	0.0003312	Paxs	534.76	Joback Method
hfust	31.66	kJ/mol	440.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83056&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

hfust:	Enthalpy of fusion at a given temperature
hvac:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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