BENZENEACETIC ACID, 2-[(2,6-DICHLOROPHENYL)AMINO]-

Other names: (2-((2,6-dichlorophenyl)amino)phenyl)acetic acid
2-[(2,6-Dichlorophenyl)amino]benzeneacetic acid
2-[(2,6-Dichlorophenyl)amino]benzoic acid (diclofenac acid)
Acetic acid, (o-(2,6-dichloroanilino)phenyl)-
Dichlofenac
diclofenac
diclofenac acid

Inchi: InChI=1S/C14H11Cl2NO2/c15-10-5-3-6-11(16)14(10)17-12-7-2-1-4-9(12)8-13(18)19/h1-

InchiKey: DCOPUUMXTXDBNB-UHFFFAOYSA-N

Formula: C14H11Cl2NO2

SMILES: O=C(O)Cc1ccccc1Nc1c(Cl)cccc1Cl

Mol. weight [g/mol]: 296.15

Physical Properties

Property code	Value	Unit	Source
hfus	38.11	kJ/mol	Joback Method
hsub	115.60 ± 1.30	kJ/mol	NIST Webbook
ie	7.45	eV	Cheméo Relay (1.0)
log10ws	-5.46		Aqueous Solubility Prediction Method
log10ws	-5.10		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	4.364		Crippen Method
mcvol	202.500	ml/mol	McGowan Method
tf	436.53	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.01	J/mol×K	859.10	Joback Method
cpg	536.14	J/mol×K	897.81	Joback Method
cpg	544.47	J/mol×K	936.52	Joback Method
cpg	552.06	J/mol×K	975.23	Joback Method

cpg	558.96	J/mol×K	1013.94	Joback Method
cpg	565.23	J/mol×K	1052.64	Joback Method
cpg	570.92	J/mol×K	1091.35	Joback Method
hfust	40.40	kJ/mol	452.60	NIST Webbook
hfust	39.40	kJ/mol	454.20	NIST Webbook
hsubt	114.70 ± 1.30	kJ/mol	339.00	NIST Webbook

Sources

Solubility Measurement of Diclofenac Acid in the Supercritical CO2: https://www.doi.org/10.1021/je200012x

Cheméo Relay (1.0):

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Solubilities of Organic Semiconductors and Nonsteroidal Anti-inflammatory Drugs in Pure and Mixed Organic Solvents: Measurement and Modeling with Hansen Solubility Parameter: https://www.doi.org/10.1021/acs.jced.8b00536

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15307865&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point