BACLOFEN

Other names: (.+/-.)-Baclofen
(.+/-.)-Baklofen
4-Amino-3-(4-chlorophenyl)butyric acid
4-Amino-3-(p-chlorophenyl)butyric acid
Ba 34647
Baclon
Benzenepropanoic acid, «beta»-(aminomethyl)-4-chloro-
Butanoic acid, 4-amino-3-(4-chlorophenyl)-
C 34647Ba
CIBA 34,647-Ba
DL-4-Amino-3-p-chlorophenylbutanoic acid
DL-Baclofen
Hydrocinnamic acid, «beta»-(aminomethyl)-p-chloro-
Lioresal
«beta»-(4-Chlorophenyl)gaba
«beta»-(Aminomethyl)-4-chlorobenzenepropanoic acid
«beta»-(Aminomethyl)-p-chlorohydrocinnamic acid
«beta»-(p-Chlorophenyl)-«gamma»-aminobutyric acid
«gamma»-Amino-«beta»-(p-chlorophenyl)butyric acid

Inchi: InChI=1S/C10H12ClNO2/c11-9-3-1-7(2-4-9)8(6-12)5-10(13)14/h1-4,8H,5-6,12H2,(H,13,1

InchiKey: KPYSYYIEGFHWSV-UHFFFAOYSA-N

Formula: C10H12ClNO2

SMILES: NCC(CC(=O)O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 213.66

Physical Properties

Property code	Value	Unit	Source
hfus	26.87	kJ/mol	Joback Method
log10ws	-1.78		Aqueous Solubility Prediction Method
log10ws	-1.70		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.857		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
rinpol	2018.10		NIST Webbook
rinpol	2018.10		NIST Webbook

tf	480.48	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.48	J/mol×K	715.43	Joback Method
cpg	414.47	J/mol×K	751.37	Joback Method
cpg	423.74	J/mol×K	787.31	Joback Method
cpg	432.35	J/mol×K	823.24	Joback Method
cpg	440.32	J/mol×K	859.18	Joback Method
cpg	447.70	J/mol×K	895.12	Joback Method
cpg	454.51	J/mol×K	931.06	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1134470&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point