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-
Benzenepropanoic acid, Â«betaÂ»-(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-
Hydrocinnamic acid, Â«betaÂ»-(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
Â«betaÂ»-(4-Chlorophenyl)gaba
Â«betaÂ»-(Aminomethyl)-4-chlorobenzenepropanoic acid
Â«betaÂ»-(Aminomethyl)-p-chlorohydrocinnamic acid
Â«betaÂ»-(p-Chlorophenyl)-Â«gammaÂ»-aminobutyric acid
Â«gammaÂ»-Amino-Â«betaÂ»-(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

CAS: 1134-47-0

Physical Properties

Property code	Value	Unit	Source
gf	-77.56	kJ/mol	Joback Method

hf	-276.71	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	78.86	kJ/mol	Joback Method
log10ws	-1.70		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.78		Aqueous Solubility Prediction Method
logp	1.857		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	2018.10		NIST Webbook
rinpol	2018.10		NIST Webbook
tb	715.43	K	Joback Method
tc	931.06	K	Joback Method
tf	480.48	K	Aqueous Solubility Prediction Method
vc	0.585	m3/kmol	Joback 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

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/

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1134470&Units=SI

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

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

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/24-906-9/Baclofen.pdf
Generated by Cheméo on 2024-04-25 17:31:15.412914636 +0000 UTC m=+16355524.333491951.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.