Chlorambucil

Other names:
Benzenebutanoic acid, 4-[bis(2-chloroethyl)amino]-
Butyric acid, 4-[p-[bis(2-chloroethyl)amino]phenyl]-
«gamma»-[p-Di(2-chloroethyl)aminophenyl]butyric acid
Ambochlorin
Amboclorin
Chloraminophene
Chlorbutin
Chloroambucil
Chlorobutine
CB 1348
Ecloril
Leukeran
Leukersan
Leukoran
Linfolizin
Linfolysin
NSC 3088
4-[p-[Bis(2-Chloroethyl)amino]phenyl]butyric acid
4-[Bis(2-chloroethyl)amino]phenylbutyric acid
«gamma»-(p-bis(2-chloroethyl)aminophenyl)butyricacid
p-(N,N-Di-2-chloroethyl)aminophenyl butyric acid
p-N,N-Di-(«beta»-chloroethyl)aminophenyl butyric acid
Cb l348
Chloraminophen
Chlorbutine
Chlorobutin
Elcoril
N,N-Di-2-chloroethyl-«gamma»-p-aminophenylbutyric acid
NCI-C03485
Phenylbutyric acid nitrogen mustard
4-(p-Bis(«beta»-chloroethyl)aminophenyl)butyric acid
4-(Bis(2-chloroethyl)amino)benzenebutanoic acid
Butanoic acid, 4-(bis(2-chloroethyl)amino)benzene-
Kyselina 4-(N,N-bis-(2-chlorethyl)-p-aminofenyl)maselna
Phenylbuttersaeure-lost
Rcra waste number U035
Leukeran tablets
4[p-[bis(2-chloroethyl)amino]benzene]butanoic acid

Inchi: InChI=1S/C14H19Cl2NO2/c15-8-10-17(11-9-16)13-6-4-12(5-7-13)2-1-3-14(18)19/h4-7H,

InchiKey: JCKYGMPEJWAADB-UHFFFAOYSA-N

Formula: C14H19Cl2NO2
SMILES: O=C(O)CCCc1ccc(N(CCCl)CCCl)cc1
Mol. weight [g/mol]: 304.21
CAS: 305-03-3

Physical Properties

Property code	Value	Unit	Source
gf	-9.04	kJ/mol	Joback Method
hf	-335.99	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	83.93	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.378		Crippen Method
mcvol	226.260	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
tb	784.73	K	Joback Method
tc	983.94	K	Joback Method
tf	340.08 ± 0.20	K	NIST Webbook
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.56	J/mol×K	784.73	Joback Method
cpg	629.45	J/mol×K	817.93	Joback Method
cpg	640.57	J/mol×K	851.13	Joback Method
cpg	650.98	J/mol×K	884.33	Joback Method
cpg	660.71	J/mol×K	917.53	Joback Method
cpg	669.83	J/mol×K	950.74	Joback Method
cpg	678.36	J/mol×K	983.94	Joback Method
hfust	29.18	kJ/mol	338.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C305033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
hfust:	Enthalpy of fusion at a given temperature
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