Benzoic acid, 4-amino-2-chloro-, 2-(diethylamino)ethyl ester

Other names: Chloroprocaine
2-(Diethylamino)ethyl 4-amino-2-chlorobenzoate
2-Chloroprocaine
Chlorprocaine
Halestyn
Piocaine
Chloroprocain

Inchi: InChI=1S/C13H19ClN2O2/c1-3-16(4-2)7-8-18-13(17)11-6-5-10(15)9-12(11)14/h5-6,9H,3

InchiKey: VDANGULDQQJODZ-UHFFFAOYSA-N

Formula: C13H19ClN2O2

SMILES: CCN(CC)CCOC(=O)c1ccc(N)cc1Cl

Mol. weight [g/mol]: 270.75

CAS: 133-16-4

Physical Properties

Property code	Value	Unit	Source
gf	83.11	kJ/mol	Joback Method
hf	-257.28	kJ/mol	Joback Method
hfus	37.89	kJ/mol	Joback Method
hvap	74.36	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.421		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	732.17	K	Joback Method
tc	944.85	K	Joback Method
tf	505.54	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	571.72	J/mol×K	732.17	Joback Method
cpg	585.62	J/mol×K	767.62	Joback Method
cpg	598.58	J/mol×K	803.06	Joback Method
cpg	610.66	J/mol×K	838.51	Joback Method
cpg	621.87	J/mol×K	873.96	Joback Method
cpg	632.25	J/mol×K	909.41	Joback Method
cpg	641.82	J/mol×K	944.85	Joback Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C133164&Units=SI

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