Benzoic acid, 4-amino-3-butoxy-, 2-(diethylamino)ethyl ester

Other names: Oxybuprocaine
Benoxinate
4-Amino-3-n-butoxy-benzoesaeure-diaethylaminoaethylester
Benoxil
Conjucain
2-(Diethylamino)ethyl 4-amino-3-butoxybenzoate
Dorsacain
Novesinol
Oxibuprokain
Oxybucaine
Oxyriprocaine
Prescaina
S 749
4-Amino-3-butoxybenzoic acid 2-diethylaminoethyl ester

Inchi: InChI=1S/C17H28N2O3/c1-4-7-11-21-16-13-14(8-9-15(16)18)17(20)22-12-10-19(5-2)6-3

InchiKey: CMHHMUWAYWTMGS-UHFFFAOYSA-N

Formula: C17H28N2O3

SMILES: CCCCOc1cc(C(=O)OCCN(CC)CC)ccc1N

Mol. weight [g/mol]: 308.42

CAS: 99-43-4

Physical Properties

Property code	Value	Unit	Source
gf	23.72	kJ/mol	Joback Method
hf	-456.32	kJ/mol	Joback Method
hfus	45.24	kJ/mol	Joback Method
hvap	81.29	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.946		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	2393.00		NIST Webbook
rinpol	2471.00		NIST Webbook
rinpol	2392.00		NIST Webbook
rinpol	2471.00		NIST Webbook
rinpol	2393.00		NIST Webbook
rinpol	2388.00		NIST Webbook

tb	808.68	K	Joback Method
tc	1010.19	K	Joback Method
tf	542.93	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.30	J/mol×K	808.68	Joback Method
cpg	811.15	J/mol×K	842.26	Joback Method
cpg	825.94	J/mol×K	875.85	Joback Method
cpg	839.69	J/mol×K	909.43	Joback Method
cpg	852.43	J/mol×K	943.02	Joback Method
cpg	864.18	J/mol×K	976.60	Joback Method
cpg	874.95	J/mol×K	1010.19	Joback Method

Sources

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=C99434&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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