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

Other names: 3-Amino-4-propoxybenzoic acid 2-(diethylamino)ethyl ester
2-(Diethylamino)ethyl 3-amino-4-propoxybenzoate
«beta»-(Diethylamino)ethyl 4-n-propoxybenzoate
Proparacaine
Proxymetacaine

Inchi: InChI=1S/C16H26N2O3/c1-4-10-20-15-8-7-13(12-14(15)17)16(19)21-11-9-18(5-2)6-3/h7

InchiKey: KCLANYCVBBTKTO-UHFFFAOYSA-N

Formula: C16H26N2O3

SMILES: CCCOc1ccc(C(=O)OCCN(CC)CC)cc1N

Mol. weight [g/mol]: 294.39

CAS: 499-67-2

Physical Properties

Property code	Value	Unit	Source
gf	15.30	kJ/mol	Joback Method
hf	-435.68	kJ/mol	Joback Method
hfus	42.65	kJ/mol	Joback Method
hvap	79.06	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.556		Crippen Method
mcvol	245.810	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	785.80	K	Joback Method
tc	988.00	K	Joback Method
tf	531.66	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.96	J/mol×K	785.80	Joback Method
cpg	753.56	J/mol×K	819.50	Joback Method

cpg	768.14	J/mol×K	853.20	Joback Method
cpg	781.72	J/mol×K	886.90	Joback Method
cpg	794.31	J/mol×K	920.60	Joback Method
cpg	805.94	J/mol×K	954.30	Joback Method
cpg	816.62	J/mol×K	988.00	Joback Method

Sources

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=C499672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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