1-Propanol, 3-(diethylamino)-2,2-dimethyl-, p-aminobenzoate (ester)

Other names: Dimethocaine
Larocaine
1-Propanol, 3-(diethylamino)-2,2-dimethyl-, p-aminobenzoate
1-Propanol, 3-(diethylamino)-2,2-dimethyl-, 4-aminobenzoate (ester)
3-(Dimethylamino)-2,2-dimethyl-1-propanol p-aminobenzoate

Inchi: InChI=1S/C16H26N2O2/c1-5-18(6-2)11-16(3,4)12-20-15(19)13-7-9-14(17)10-8-13/h7-10

InchiKey: OWQIUQKMMPDHQQ-UHFFFAOYSA-N

Formula: C16H26N2O2

SMILES: CCN(CC)CC(C)(C)COC(=O)c1ccc(N)cc1

Mol. weight [g/mol]: 278.39

CAS: 94-15-5

Physical Properties

Property code	Value	Unit	Source
gf	132.77	kJ/mol	Joback Method
hf	-300.74	kJ/mol	Joback Method
hfus	34.44	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.794		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	755.17	K	Joback Method
tc	965.61	K	Joback Method
tf	499.33	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.05	J/mol×K	755.17	Joback Method
cpg	728.54	J/mol×K	790.24	Joback Method

cpg	743.92	J/mol×K	825.32	Joback Method
cpg	758.26	J/mol×K	860.39	Joback Method
cpg	771.61	J/mol×K	895.47	Joback Method
cpg	784.05	J/mol×K	930.54	Joback Method
cpg	795.63	J/mol×K	965.61	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=C94155&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