DIMETHOCAINE

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]:	278.40

Physical Properties

Property code	Value	Unit	Source
hfus	34.44	kJ/mol	Joback Method
ie	7.29	eV	Cheméo Relay (1.0)
log10ws	-3.30		Cheméo Relay (1.0)
logp	2.794		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	634.33	K	Cheméo Relay (1.0)
tf	344.81	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94155&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point