PROPOXYCAINE

Other names:	4-Amino-2-propoxybenzoic acid, 2-(diethylamino)ethyl ester
	Blockain
	2-Diethylaminoethyl 4-amino-2-propoxybenzoate
	2-Diethylaminoethyl 4-amino-2-propoxybenzoic acid ester
	2'-Diethylaminoethyl 2-propoxy-4-aminobenzoate
	Pravocaine
	Propoxycaine
	Ranocaine
Inchi:	InChI=1S/C16H26N2O3/c1-4-10-20-15-12-13(17)7-8-14(15)16(19)21-11-9-18(5-2)6-3/h7
InchiKey:	CAJIGINSTLKQMM-UHFFFAOYSA-N
Formula:	C16H26N2O3
SMILES:	CCCOc1cc(N)ccc1C(=O)OCCN(CC)CC
Mol. weight [g/mol]:	294.39

Physical Properties

Property code	Value	Unit	Source
hf	-552.94	kJ/mol	Cheméo Relay (1.0)
hfus	42.65	kJ/mol	Joback Method
hvap	87.96	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.00		Cheméo Relay (1.0)
logp	2.556		Crippen Method
mcvol	245.810	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
tb	652.66	K	Cheméo Relay (1.0)
tf	294.40	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86431&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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point