MEXILETINE

Other names:	2-Propanamine, 1-(2,6-dimethylphenoxy)- Ethylamine, 1-methyl-2-(2,6-xylyloxy)- 1-(2,6-Dimethylphenoxy)-2-aminopropane 1-(2',6'-Dimethylphenoxy)-2-aminopropane 1-Methyl-2-(2,6-xylyloxy)ethylamine 1-(2,6-Dimethylphenoxy)-2-propanamine Mexiletina 2-Amino-1-(2,6-dimethylphenoxy)propane 5370-01-4 Mexilitine
Inchi:	InChI=1S/C11H17NO/c1-8-5-4-6-9(2)11(8)13-7-10(3)12/h4-6,10H,7,12H2,1-3H3
InchiKey:	VLPIATFUUWWMKC-UHFFFAOYSA-N
Formula:	C11H17NO
SMILES:	Cc1cccc(C)c1OCC(C)N
Mol. weight [g/mol]:	179.26

Physical Properties

Property code	Value	Unit	Source
hfus	20.37	kJ/mol	Joback Method
ie	8.38	eV	Cheméo Relay (1.0)
logp	2.029		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
rinpol	1408.00		NIST Webbook
tb	527.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.03	J/mol×K	582.23	Joback Method
cpg	403.25	J/mol×K	618.30	Joback Method
cpg	417.65	J/mol×K	654.37	Joback Method
cpg	431.25	J/mol×K	690.44	Joback Method
cpg	444.07	J/mol×K	726.51	Joback Method
cpg	456.12	J/mol×K	762.58	Joback Method

cpg	467.41	J/mol×K	798.66	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31828714&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
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature