

Mexiletine acetate

Other names:	MEXILETINE, AC
Inchi:	InChI=1S/C13H19NO2/c1-9-6-5-7-10(2)13(9)16-8-11(3)14-12(4)15/h5-7,11H,8H2,1-4H3
InchiKey:	DNSFMKGQWLZMOJ-UHFFFAOYSA-N
Formula:	C13H19NO2
SMILES:	CC(=O)NC(C)COc1c(C)cccc1C
Mol. weight [g/mol]:	221.30

Physical Properties

Property code	Value	Unit	Source
gf	4.76	kJ/mol	Joback Method
hf	-294.67	kJ/mol	Joback Method
hfus	27.05	kJ/mol	Joback Method
hvap	63.34	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.207		Crippen Method
mvol	187.690	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1780.00		NIST Webbook
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tb	659.50	K	Joback Method
tc	868.12	K	Joback Method
tf	397.55	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.39	J/molxK	659.50	Joback Method
cpg	511.74	J/molxK	694.27	Joback Method
cpg	526.20	J/molxK	729.04	Joback Method
cpg	539.79	J/molxK	763.81	Joback Method
cpg	552.52	J/molxK	798.58	Joback Method
cpg	564.42	J/molxK	833.35	Joback Method
cpg	575.50	J/molxK	868.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U120152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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