

MEXILETINE, M(DESAMINO-OXO-)

Inchi:	InChI=1S/C11H14O2/c1-8-5-4-6-9(2)11(8)13-7-10(3)12/h4-6H,7H2,1-3H3
InchiKey:	XDJJULAUHYAJQBU-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CC(=O)COc1c(C)cccc1C
Mol. weight [g/mol]:	178.23

Physical Properties

Property code	Value	Unit	Source
gf	-99.03	kJ/mol	Joback Method
hf	-301.58	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	52.84	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.271		Crippen Method
mvol	149.530	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
tb	564.01	K	Joback Method
tc	775.37	K	Joback Method
tf	337.35	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.82	J/molxK	564.01	Joback Method
cpg	359.69	J/molxK	599.24	Joback Method
cpg	372.86	J/molxK	634.46	Joback Method
cpg	385.33	J/molxK	669.69	Joback Method
cpg	397.11	J/molxK	704.92	Joback Method
cpg	408.21	J/molxK	740.15	Joback Method
cpg	418.63	J/molxK	775.37	Joback Method
dvisc	0.0013555	Paxs	337.35	Joback Method

dvisc	0.0008295	Paxs	375.13	Joback Method
dvisc	0.0005553	Paxs	412.90	Joback Method
dvisc	0.0003976	Paxs	450.68	Joback Method
dvisc	0.0002998	Paxs	488.46	Joback Method
dvisc	0.0002354	Paxs	526.23	Joback Method
dvisc	0.0001909	Paxs	564.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255246&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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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

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