MEXILETINE, M(HO-) ISOMER 2, AC

Inchi: InChI=1S/C15H21NO4/c1-9-6-14(20-13(5)18)7-10(2)15(9)19-8-11(3)16-12(4)17/h6-7,11H
InchiKey: XPSPCVHEVQZZIQ-UHFFFAOYSA-N
Formula: C15H21NO4
SMILES: CC(=O)NC(C)COc1c(C)cc(OC(C)=O)cc1C
Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
gf	-221.95	kJ/mol	Joback Method
hf	-592.22	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	77.61	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	2.132		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	786.53	K	Joback Method
tc	995.72	K	Joback Method
tf	504.77	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.27	J/mol×K	786.53	Joback Method
cpg	661.40	J/mol×K	821.40	Joback Method
cpg	674.52	J/mol×K	856.26	Joback Method
cpg	686.64	J/mol×K	891.13	Joback Method
cpg	697.75	J/mol×K	925.99	Joback Method
cpg	707.86	J/mol×K	960.86	Joback Method
cpg	716.96	J/mol×K	995.72	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255291&Units=SI
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
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:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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