Moprolol

Inchi: InChI=1S/C13H21NO3/c1-10(2)14-8-11(15)9-17-13-7-5-4-6-12(13)16-3/h4-7,10-11,14-15
InchiKey: LFTFGCDECFPSQD-UHFFFAOYSA-N
Formula: C13H21NO3
SMILES: COc1ccccc1OCC(O)CNC(C)C
Mol. weight [g/mol]: 239.31
CAS: 5741-22-0

Physical Properties

Property code	Value	Unit	Source
gf	-100.95	kJ/mol	Joback Method
hf	-460.35	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	74.63	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.433		Crippen Method
mcvol	197.860	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1802.00		NIST Webbook
rinpol	1802.00		NIST Webbook
tb	714.81	K	Joback Method
tc	907.62	K	Joback Method
tf	403.15	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.23	J/mol×K	714.81	Joback Method
cpg	579.22	J/mol×K	746.95	Joback Method
cpg	592.41	J/mol×K	779.08	Joback Method
cpg	604.80	J/mol×K	811.22	Joback Method
cpg	616.40	J/mol×K	843.35	Joback Method
cpg	627.23	J/mol×K	875.49	Joback Method
cpg	637.30	J/mol×K	907.62	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=C5741220&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

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