

Etodroxine hydrolized, acetylated

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H13ClO2/c1-11(17)18-15(12-5-3-2-4-6-12)13-7-9-14(16)10-8-13/h2-10,15H

FLBMKFDKDSWBQG-UHFFFAOYSA-N

C15H13ClO2

CC(=O)OC(c1ccccc1)c1ccc(Cl)cc1

260.72

Physical Properties

Property code	Value	Unit	Source
gf	42.32	kJ/mol	Joback Method
hf	-157.16	kJ/mol	Joback Method
hfus	25.76	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.993		Crippen Method
mcvol	194.370	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	714.22	K	Joback Method
tc	960.09	K	Joback Method
tf	411.25	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.72	J/mol×K	714.22	Joback Method
cpg	506.28	J/mol×K	755.20	Joback Method
cpg	519.60	J/mol×K	796.18	Joback Method
cpg	531.74	J/mol×K	837.16	Joback Method
cpg	542.75	J/mol×K	878.14	Joback Method
cpg	552.70	J/mol×K	919.12	Joback Method

cpg	561.64	J/mol×K	960.09	Joback Method
dvisc	0.0012667	Pa×s	411.25	Joback Method
dvisc	0.0006843	Pa×s	461.75	Joback Method
dvisc	0.0004174	Pa×s	512.24	Joback Method
dvisc	0.0002782	Pa×s	562.74	Joback Method
dvisc	0.0001982	Pa×s	613.23	Joback Method
dvisc	0.0001487	Pa×s	663.73	Joback Method
dvisc	0.0001162	Pa×s	714.22	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=R536362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	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:	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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