(.+/-.)-Baclofen, N-dimethylaminomethylene-, ethyl ester

Inchi: InChI=1S/C15H21ClN2O2/c1-4-20-15(19)9-13(10-17-11-18(2)3)12-5-7-14(16)8-6-12/h5-

InchiKey: ZSKUIAQDRSXQEP-UHFFFAOYSA-N

Formula: C15H21ClN2O2

SMILES: CCOC(=O)CC(CN=CN(C)C)c1ccc(Cl)cc1

Mol. weight [g/mol]: 296.79

Physical Properties

Property code	Value	Unit	Source
hf	-243.94	kJ/mol	Joback Method
hvap	70.43	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.967		Crippen Method
mcvol	233.790	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	2108.00		NIST Webbook
tb	776.66	K	Joback Method
tc	992.48	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375702&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

hf: Enthalpy of formation 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