

Iproclozide

Inchi:	InChI=1S/C11H15ClN2O2/c1-8(2)13-14-11(15)7-16-10-5-3-9(12)4-6-10/h3-6,8,13H,7H2,
InchiKey:	GGECDTUJZOXAAR-UHFFFAOYSA-N
Formula:	C11H15ClN2O2
SMILES:	CC(C)NNC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	242.71
CAS:	3544-35-2

Physical Properties

Property code	Value	Unit	Source
hfus	31.56	kJ/mol	Joback Method
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-2.72		Cheméo Relay (1.0)
logp	1.748		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
tb	581.67	K	Cheméo Relay (1.0)
tf	366.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.49310e+01
Coeff. B	9.84340e-01
Coeff. C	-5.29860e-04
Coeff. D	8.59600e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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