

Benmoxin

Inchi:	InChI=1S/C15H16N2O/c1-12(13-8-4-2-5-9-13)16-17-15(18)14-10-6-3-7-11-14/h2-12,16H
InchiKey:	BEWNZPMDJIGBED-UHFFFAOYSA-N
Formula:	C15H16N2O
SMILES:	CC(NNC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	240.31
CAS:	7654-03-7

Physical Properties

Property code	Value	Unit	Source
hf	35.91	kJ/mol	Cheméo Relay (1.0)
hfus	30.96	kJ/mol	Joback Method
hvap	104.43	kJ/mol	Cheméo Relay (1.0)
ie	8.70	eV	Cheméo Relay (1.0)
log10ws	-2.86		Cheméo Relay (1.0)
logp	2.682		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
tb	610.86	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	-7.53000e+01
Coeff. B	1.40132e+00
Coeff. C	-9.36300e-04
Coeff. D	2.29760e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Sources

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
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

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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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