

5-phenyl-4,5-dihydro-1,3-oxazol-2-amine

Inchi:	InChI=1S/C9H10N2O/c10-9-11-6-8(12-9)7-4-2-1-3-5-7/h1-5,8H,6H2,(H2,10,11)
InchiKey:	SYAKTDIEAPMBAL-UHFFFAOYSA-N
Formula:	C9H10N2O
SMILES:	NC1=NCC(c2ccccc2)O1
Mol. weight [g/mol]:	162.19
CAS:	2207-50-3

Physical Properties

Property code	Value	Unit	Source
hfus	26.19	kJ/mol	Joback Method
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-2.01		Cheméo Relay (1.0)
logp	1.073		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
tb	535.22	K	Cheméo Relay (1.0)
tf	409.40	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	-4.68700e+01
Coeff. B	8.88480e-01
Coeff. C	-4.98900e-04
Coeff. D	8.15000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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