

2-(pyridine-3-carbonylamino)ethyl nitrate

Inchi:	InChI=1S/C8H9N3O4/c12-8(7-2-1-3-9-6-7)10-4-5-15-11(13)14/h1-3,6H,4-5H2,(H,10,12)
InchiKey:	LBHIOVVIQHISOQN-UHFFFAOYSA-N
Formula:	C8H9N3O4
SMILES:	O=C(NCCO[N+](=O)[O-])c1cccn1
Mol. weight [g/mol]:	211.18
CAS:	65141-46-0

Physical Properties

Property code	Value	Unit	Source
hf	-143.43	kJ/mol	Cheméo Relay (1.0)
hvap	94.89	kJ/mol	Cheméo Relay (1.0)
ie	9.90	eV	Cheméo Relay (1.0)
log10ws	-1.52		Cheméo Relay (1.0)
logp	0.020		Crippen Method
mcvol	144.640	ml/mol	McGowan Method
tb	577.28	K	Cheméo Relay (1.0)
tf	365.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
t_b:	Normal Boiling Point Temperature
t_f:	Normal melting (fusion) point

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