ETHYL 3-PYRIDYLACETATE

Other names: 3-Pyridineacetic acid, ethyl ester
Acetic acid, 2-(3-pyridyl)-, ethyl ester
Ethyl 3-pyridineacetate
Inchi: InChI=1S/C9H11NO2/c1-2-12-9(11)6-8-4-3-5-10-7-8/h3-5,7H,2,6H2,1H3
InchiKey: RPWXYCRIAGBAGY-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: CCOC(=O)Cc1cccnc1
Mol. weight [g/mol]: 165.19

Physical Properties

Property code	Value	Unit	Source
af	0.4939		Cheméo Relay (1.0)
hvap	65.82	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	Cheméo Relay (1.0)
log10ws	-0.51		Cheméo Relay (1.0)
logp	1.187		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	2977.42	kPa	Cheméo Relay (1.0, beta)
tb	514.95	K	Cheméo Relay (1.0)
tc	735.46	K	Cheméo Relay (1.0)
tf	267.66	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	0.05	NIST Webbook

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39931776&Units=SI

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point