3-AMINO-4-CARBETHOXYPYRAZOLE

Other names:	3-Amino-4-ethoxycarbonylpyrazole
	Ethyl 3-amino-4-pyrazolecarboxylate
	Ethyl 3-aminopyrazole-4-carboxylate
	1H-Pyrazole-4-carboxylic acid, 3-amino-, ethyl ester
	ethyl 3-amino-1H-pyrazole-4-carboxylate
Inchi:	InChI=1S/C6H9N3O2/c1-2-11-6(10)4-3-8-9-5(4)7/h3H,2H2,1H3,(H3,7,8,9)
InchiKey:	YPXGHKWOJXQLQU-UHFFFAOYSA-N
Formula:	C6H9N3O2
SMILES:	CCOC(=O)c1c[nH]nc1N
Mol. weight [g/mol]:	155.16

Physical Properties

Property code	Value	Unit	Source
hf	-271.96	kJ/mol	Cheméo Relay (1.0)
hvap	79.73	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	Cheméo Relay (1.0)
log10ws	-2.32		Cheméo Relay (1.0)
logp	-0.313		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3453.95	kPa	Cheméo Relay (1.0, beta)
tb	580.94	K	Cheméo Relay (1.0)
tf	459.79	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6994258&Units=SI
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):	

Legend

hf:	Enthalpy of formation 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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point