CH3NCCCO

Inchi: InChI=1S/C4H3NO/c1-5-3-2-4-6/h1H3
InchiKey: TYRNLNDZPWBIKE-UHFFFAOYSA-N
Formula: C4H3NO
SMILES: CN=C=C=C=O
Mol. weight [g/mol]: 81.07
CAS: 145355-49-3

Physical Properties

Property code	Value	Unit	Source
affp	920.00	kJ/mol	NIST Webbook
basg	887.50	kJ/mol	NIST Webbook
hf	194.26	kJ/mol	Joback Method
hvap	34.90	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	-0.171		Crippen Method
mcvol	65.870	ml/mol	McGowan Method
pc	5536.07	kPa	Joback Method
tb	364.13	K	Joback Method
tc	569.19	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C145355493&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

affp: Proton affinity

basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tc:	Critical Temperature

Latest version available from:
https://www.chemeo.com/cid/87-982-6/CH3NCCCO.pdf
Generated by Cheméo on 2024-04-29 23:31:20.913442207 +0000 UTC m=+16722729.834019523.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.