4-Acetamidophenylacetonitrile

Inchi: InChI=1S/C10H10N2O/c1-8(13)12-10-4-2-9(3-5-10)6-7-11/h2-5H,6H2,1H3,(H,12,13)
InchiKey: SPAOQNOLRMENDZ-UHFFFAOYSA-N
Formula: C10H10N2O
SMILES: CC(O)=Nc1ccc(CC#N)cc1
Mol. weight [g/mol]: 174.20
CAS: 25025-06-3

Physical Properties

Property code	Value	Unit	Source
hf	60.41	kJ/mol	Joback Method
hvap	71.34	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.361		Crippen Method
mcvol	140.930	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
tb	730.68	K	Joback Method
tc	954.90	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25025063&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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/85-975-6/4-Acetamidophenylacetonitrile.pdf
Generated by Cheméo on 2025-12-23 01:18:22.061532981 +0000 UTC m=+6200899.591573645.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.