

4-AMINO BENZOYLACETONITRILE

Other names:	Benzenepropanenitrile, 4-amino-«beta»-oxo-Propionitrile, 3-(4-aminophenyl)-3-oxo-(p-Aminobenzoyl)acetonitrile
Inchi:	InChI=1S/C9H8N2O/c10-6-5-9(12)7-1-3-8(11)4-2-7/h1-4H,5,11H2
InchiKey:	BEWGVKVVWWKCFHO-UHFFFAOYSA-N
Formula:	C9H8N2O
SMILES:	N#CCC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	160.18

Physical Properties

Property code	Value	Unit	Source
hf	66.88	kJ/mol	Cheméo Relay (1.0)
hfus	21.02	kJ/mol	Joback Method
ie	8.31	eV	Cheméo Relay (1.0)
log10ws	-1.58		Cheméo Relay (1.0)
logp	1.365		Crippen Method
mcvol	126.840	ml/mol	McGowan Method
tb	623.05	K	Cheméo Relay (1.0)
tf	437.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.07	J/mol×K	665.46	Joback Method
cpg	313.71	J/mol×K	705.96	Joback Method
cpg	322.60	J/mol×K	746.45	Joback Method
cpg	330.78	J/mol×K	786.95	Joback Method
cpg	338.29	J/mol×K	827.45	Joback Method
cpg	345.15	J/mol×K	867.94	Joback Method
cpg	351.42	J/mol×K	908.44	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C59443946&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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