

2-AZETIDINECARBOXYLIC ACID

Other names:	L-pyrrolidine-2-carboxylic acid
Inchi:	InChI=1S/C4H7NO2/c6-4(7)3-1-2-5-3/h3,5H,1-2H2,(H,6,7)
InchiKey:	IADUEWIBXOCDZ-UHFFFAOYSA-N
Formula:	C4H7NO2
SMILES:	O=C(O)C1CCN1
Mol. weight [g/mol]:	101.10

Physical Properties

Property code	Value	Unit	Source
hf	-324.72	kJ/mol	Cheméo Relay (1.0)
hfus	17.43	kJ/mol	Joback Method
ie	9.18	eV	Cheméo Relay (1.0)
logp	-0.567		Crippen Method
mcvol	73.780	ml/mol	McGowan Method
tb	492.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.96	J/mol×K	496.53	Joback Method
cpg	169.32	J/mol×K	530.16	Joback Method
cpg	177.23	J/mol×K	563.79	Joback Method
cpg	184.70	J/mol×K	597.42	Joback Method
cpg	191.75	J/mol×K	631.05	Joback Method
cpg	198.39	J/mol×K	664.68	Joback Method
cpg	204.65	J/mol×K	698.30	Joback Method

Sources

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=C2517046&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>

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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