

N-Formylpyrrolidine

Other names:	N-Formylpyrrolidine 1-Formylpyrrolidine Prolinal pyrrolidine-1-carbaldehyde
Inchi:	InChI=1S/C5H9NO/c7-5-6-3-1-2-4-6/h5H,1-4H2
InchiKey:	AGRIQBHIKABLPJ-UHFFFAOYSA-N
Formula:	C5H9NO
SMILES:	O=CN1CCCC1
Mol. weight [g/mol]:	99.13

Physical Properties

Property code	Value	Unit	Source
ie	9.38	eV	Cheméo Relay (1.0)
logp	0.239		Crippen Method
mcvol	82.000	ml/mol	McGowan Method
pc	5282.14	kPa	Cheméo Relay (1.0, beta)
ripol	1691.00		NIST Webbook
tb	482.72	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.50 ± 1.50	K	2.30	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3760541&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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