

1-Piperidinecarboxaldehyde

Other names:	Formylpiperidine N-Formylpiperidine Piperidine, 1-formyl- Piperidinoformamide 1-Formylpiperidine N-Formylpiperidin Formyl piperidide piperidine-N-carbaldehyde
Inchi:	InChI=1S/C6H11NO/c8-6-7-4-2-1-3-5-7/h6H,1-5H2
InchiKey:	FEWLNYSYJNLUOO-UHFFFAOYSA-N
Formula:	C6H11NO
SMILES:	O=CN1CCCCC1
Mol. weight [g/mol]:	113.16
CAS:	2591-86-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.57		Crippen Method
logp	0.629		Crippen Method
mcvol	96.090	ml/mol	McGowan Method
rinpol	1140.10		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1140.10		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1134.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1786.00		NIST Webbook
tb	495.70	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2591868&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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