

5-OXO-PYRROLIDINE-2-CARBOXYLIC ACID, METHYL ESTER

Other names:	2-Pyrrolidone-5-carboxylic acid, methyl ester Methyl 5-oxoprolinate methyl 5-oxo-DL-prolinate
Inchi:	InChI=1S/C6H9NO3/c1-10-6(9)4-2-3-5(8)7-4/h4H,2-3H2,1H3,(H,7,8)
InchiKey:	HQGPKMSGXAUKHT-UHFFFAOYSA-N
Formula:	C6H9NO3
SMILES:	COC(=O)C1CCC(=O)N1
Mol. weight [g/mol]:	143.14

Physical Properties

Property code	Value	Unit	Source
hf	-523.00	kJ/mol	Cheméo Relay (1.0)
hfus	17.12	kJ/mol	Joback Method
hvap	76.16	kJ/mol	Cheméo Relay (1.0)
logp	-0.562		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
rinpol	1390.90		NIST Webbook
rinpol	1392.20		NIST Webbook
rinpol	1390.90		NIST Webbook
tb	544.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.27	J/mol×K	544.62	Joback Method
cpg	255.13	J/mol×K	583.30	Joback Method
cpg	267.43	J/mol×K	621.98	Joback Method
cpg	279.12	J/mol×K	660.66	Joback Method
cpg	290.17	J/mol×K	699.33	Joback Method
cpg	300.55	J/mol×K	738.01	Joback Method
cpg	310.21	J/mol×K	776.69	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54571663&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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