

DL-Proline, 5-oxo-, 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
CAS:	54571-66-3

Physical Properties

Property code	Value	Unit	Source
gf	-232.61	kJ/mol	Joback Method
hf	-451.38	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	49.37	kJ/mol	Joback Method
log10ws	-0.17		Crippen Method
logp	-0.562		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
rinpol	1392.20		NIST Webbook
rinpol	1390.90		NIST Webbook
rinpol	1390.90		NIST Webbook
tb	544.62	K	Joback Method
tc	776.69	K	Joback Method
tf	413.69	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.27	J/molxK	544.62	Joback Method
cpg	255.13	J/molxK	583.30	Joback Method
cpg	267.43	J/molxK	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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54571663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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