

4,4-DIMETHYL-2-OXAZOLIDINONE

Other names:	4,4-Dimethyl-2-oxazolidinone
Inchi:	InChI=1S/C5H9NO2/c1-5(2)3-8-4(7)6-5/h3H2,1-2H3,(H,6,7)
InchiKey:	SYARCRAQWWGZKY-UHFFFAOYSA-N
Formula:	C5H9NO2
SMILES:	CC1(C)COC(=O)N1
Mol. weight [g/mol]:	115.13

Physical Properties

Property code	Value	Unit	Source
hf	-407.53	kJ/mol	Cheméo Relay (1.0)
hfus	13.42	kJ/mol	Joback Method
hvap	63.33	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	NIST Webbook
logp	0.505		Crippen Method
mcpvol	87.870	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.45	J/mol×K	472.64	Joback Method
cpg	202.53	J/mol×K	512.22	Joback Method
cpg	213.88	J/mol×K	551.81	Joback Method
cpg	224.58	J/mol×K	591.39	Joback Method
cpg	234.72	J/mol×K	630.97	Joback Method
cpg	244.38	J/mol×K	670.55	Joback Method
cpg	253.65	J/mol×K	710.14	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=C26654397&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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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