3-Methyl-5-pyrazolone

Inchi: InChI=1S/C4H6N2O/c1-3-2-4(7)6-5-3/h2H2,1H3,(H,6,7)
InchiKey: NHLAPJMCARJFOG-UHFFFAOYSA-N
Formula: C4H6N2O
SMILES: CC1=NNC(=O)C1
Mol. weight [g/mol]: 98.10

Physical Properties

Property code	Value	Unit	Source
hfus	14.05	kJ/mol	Joback Method
logp	-0.118		Crippen Method
mcvol	73.590	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.61	J/mol×K	485.08	Joback Method
cpg	166.68	J/mol×K	526.47	Joback Method
cpg	177.36	J/mol×K	567.85	Joback Method
cpg	187.61	J/mol×K	609.24	Joback Method
cpg	197.37	J/mol×K	650.63	Joback Method
cpg	206.59	J/mol×K	692.01	Joback Method
cpg	215.21	J/mol×K	733.40	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?Str2File=C108269
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume