3(2H)-Furanone, 2,5-dimethyl-

Other names: 2H-Furan-3-one, 2,5-dimethyl
3(2H)-Furanone, 2,5-dimethyl-
2,5-dimethylfuran-3(2H)-one
Inchi: InChI=1S/C6H8O2/c1-4-3-6(7)5(2)8-4/h3,5H,1-2H3
InchiKey: ASOSVCXGWPDUGN-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CC1=CC(=O)C(C)O1
Mol. weight [g/mol]: 112.13

Physical Properties

Property code	Value	Unit	Source
hfus	13.55	kJ/mol	Joback Method
ie	9.23 ± 0.05	eV	NIST Webbook
logp	0.878		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
rinpol	918.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	913.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1483.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.89	J/mol×K	450.87	Joback Method

cpg	190.07	J/mol×K	487.66	Joback Method
cpg	200.83	J/mol×K	524.45	Joback Method
cpg	211.16	J/mol×K	561.23	Joback Method
cpg	221.04	J/mol×K	598.02	Joback Method
cpg	230.47	J/mol×K	634.81	Joback Method
cpg	239.42	J/mol×K	671.60	Joback Method

Sources

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=C14400670&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices