

3(2H)-Furanone, 4-methoxy-2,5-dimethyl-

Other names:	2,5-Dimethyl-4-methoxy-3(2H)-furanone 2,5-Dimethyl-4-methoxy-2,3-dihydro-3-furanone 2,5-Dimethyl 4-methoxy furan-3-one 3(2H)-Furanone, 2,5-dimethyl-4-methoxy Mesifuran Mesifurane 4-Methoxy-2,5-dimethyl-3(2H)-furanone 4-methoxy-2,5-dimethylfuran-3(2H)-one
Inchi:	InChI=1S/C7H10O3/c1-4-6(8)7(9-3)5(2)10-4/h4H,1-3H3
InchiKey:	SIMKGHMLPVDSJE-UHFFFAOYSA-N
Formula:	C7H10O3
SMILES:	<chem>COC1=C(C)OC(C)C1=O</chem>
Mol. weight [g/mol]:	142.15
CAS:	4077-47-8

Physical Properties

Property code	Value	Unit	Source
gf	-258.40	kJ/mol	Joback Method
hf	-494.41	kJ/mol	Joback Method
hfus	16.94	kJ/mol	Joback Method
hvap	44.22	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.852		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpola	1027.00		NIST Webbook
rinpola	1031.00		NIST Webbook
rinpola	1031.00		NIST Webbook
rinpola	1032.00		NIST Webbook
rinpola	1055.00		NIST Webbook
rinpola	1065.00		NIST Webbook
rinpola	1065.00		NIST Webbook
rinpola	1057.00		NIST Webbook
rinpola	1056.00		NIST Webbook
rinpola	1051.00		NIST Webbook
rinpola	1057.00		NIST Webbook
rinpola	1064.00		NIST Webbook

ripol	1561.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1556.00		NIST Webbook
tb	501.15	K	Joback Method
tc	717.78	K	Joback Method
tf	322.37	K	Joback Method
vc	0.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.60	J/mol×K	501.15	Joback Method
cpg	253.67	J/mol×K	537.25	Joback Method
cpg	265.35	J/mol×K	573.36	Joback Method
cpg	276.62	J/mol×K	609.46	Joback Method
cpg	287.44	J/mol×K	645.57	Joback Method
cpg	297.79	J/mol×K	681.67	Joback Method
cpg	307.63	J/mol×K	717.78	Joback Method

Sources

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=C4077478&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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