3,4-dimethylfuran

Inchi: InChI=1S/C6H8O/c1-5-3-7-4-6(5)2/h3-4H,1-2H3
InchiKey: IVHPMIPYSOTYNM-UHFFFAOYSA-N
Formula: C6H8O
SMILES: Cc1cocc1C
Mol. weight [g/mol]: 96.13
CAS: 20843-07-6

Physical Properties

Property code	Value	Unit	Source
affp	869.00	kJ/mol	NIST Webbook
basg	838.30	kJ/mol	NIST Webbook
log10ws	-6.16		Crippen Method
logp	1.896		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	724.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.20	K	96.00	NIST Webbook
tbrp	322.20	K	16.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38435e+01
Coeff. B	-2.98801e+03
Coeff. C	-3.89140e+01
Temperature range (K), min.	259.34

Temperature range (K), max.	389.13

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20843076&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure