

2-Furanmethanol, acetate

Other names:	Furfuryl alcohol, acetate Acetic acid furfurylester Furfuryl acetate 2-Acetoxyethylfuran 2-Furanmethyl acetate 2-Furfuryl-acetate Furfuryl ethanoate
Inchi:	InChI=1S/C7H8O3/c1-6(8)10-5-7-3-2-4-9-7/h2-4H,5H2,1H3
InchiKey:	CKOYRRWBOKMNRG-UHFFFAOYSA-N
Formula:	C7H8O3
SMILES:	CC(=O)OCc1ccco1
Mol. weight [g/mol]:	140.14
CAS:	623-17-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.78		Crippen Method
logp	1.343		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
rinpol	966.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	966.00		NIST Webbook

ripol	996.00	NIST Webbook
ripol	995.00	NIST Webbook
ripol	969.00	NIST Webbook
ripol	967.00	NIST Webbook
ripol	991.00	NIST Webbook
ripol	1521.00	NIST Webbook
ripol	1542.00	NIST Webbook
ripol	1539.00	NIST Webbook
ripol	1512.00	NIST Webbook
ripol	1514.00	NIST Webbook
ripol	1524.00	NIST Webbook
ripol	1542.00	NIST Webbook
ripol	1534.00	NIST Webbook
ripol	1521.00	NIST Webbook
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ripol	1518.00	NIST Webbook
ripol	1538.00	NIST Webbook
ripol	1539.00	NIST Webbook
ripol	1559.00	NIST Webbook
ripol	1514.00	NIST Webbook
ripol	1550.00	NIST Webbook
ripol	1518.00	NIST Webbook

ripol	1554.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1539.00		NIST Webbook
tb	450.20	K	NIST Webbook
tb	455.35 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	45.69	kJ/mol	454.20	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C623176&Units=SI

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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