

trans-Furfurylideneacetone

Other names: 1-(2-furanyl)-1-buten-3-one, trans
Inchi: InChI=1S/C8H8O2/c1-7(9)4-5-8-3-2-6-10-8/h2-6H,1H3/b5-4+
InchiKey: GBKGJMYPQZODMI-SNAWJCMRSA-N
Formula: C8H8O2
SMILES: CC(=O)C=Cc1ccco1
Mol. weight [g/mol]: 136.15
CAS: 41438-24-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.15		Crippen Method
logp	1.882		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
ripol	1890.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1891.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C41438248&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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