

furfural ethyl isoamyl acetal

Inchi:	InChI=1S/C13H22O2/c1-4-14-13(12-7-5-6-8-12)15-10-9-11(2)3/h5-7,11,13H,4,8-10H2,1-
InchiKey:	KZDDWXGYZGWAFF-UHFFFAOYSA-N
Formula:	C13H22O2
SMILES:	CCOC(OCCC(C)C)C1=CC=CC1
Mol. weight [g/mol]:	210.31

Physical Properties

Property code	Value	Unit	Source
gf	-61.75	kJ/mol	Joback Method
hf	-401.74	kJ/mol	Joback Method
hfus	19.68	kJ/mol	Joback Method
hvap	50.39	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.298		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
ripol	1652.00		NIST Webbook
ripol	1652.00		NIST Webbook
tb	564.05	K	Joback Method
tc	757.24	K	Joback Method
tf	279.91	K	Joback Method
vc	0.702	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.30	J/molxK	564.05	Joback Method
cpg	483.96	J/molxK	596.25	Joback Method
cpg	500.77	J/molxK	628.45	Joback Method
cpg	516.75	J/molxK	660.65	Joback Method
cpg	531.92	J/molxK	692.84	Joback Method
cpg	546.29	J/molxK	725.04	Joback Method
cpg	559.89	J/molxK	757.24	Joback Method
dvisc	0.0034362	Paxs	279.91	Joback Method

dvisc	0.0013761	Paxs	327.27	Joback Method
dvisc	0.0006946	Paxs	374.62	Joback Method
dvisc	0.0004087	Paxs	421.98	Joback Method
dvisc	0.0002677	Paxs	469.34	Joback Method
dvisc	0.0001894	Paxs	516.69	Joback Method
dvisc	0.0001421	Paxs	564.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R340864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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