

3,4,5-Trimethoxybenzyl methyl ether

Inchi:	InChI=1S/C11H16O4/c1-12-7-8-5-9(13-2)11(15-4)10(6-8)14-3/h5-6H,7H2,1-4H3
InchiKey:	MRSLZYLPFVSLDY-UHFFFAOYSA-N
Formula:	C11H16O4
SMILES:	<chem>COCc1cc(OC)c(OC)c(OC)c1</chem>
Mol. weight [g/mol]:	212.24
CAS:	75921-68-5

Physical Properties

Property code	Value	Unit	Source
gf	-294.74	kJ/mol	Joback Method
hf	-597.13	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.859		Crippen Method
mvol	165.570	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	582.38	K	Joback Method
tc	780.84	K	Joback Method
tf	366.63	K	Joback Method
vc	0.616	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.56	J/molxK	582.38	Joback Method
cpg	415.64	J/molxK	615.46	Joback Method
cpg	429.21	J/molxK	648.53	Joback Method
cpg	442.23	J/molxK	681.61	Joback Method
cpg	454.67	J/molxK	714.69	Joback Method
cpg	466.50	J/molxK	747.76	Joback Method
cpg	477.68	J/molxK	780.84	Joback Method

dvisc	0.0005294	Paxs	366.63	Joback Method
dvisc	0.0003487	Paxs	402.59	Joback Method
dvisc	0.0002459	Paxs	438.55	Joback Method
dvisc	0.0001829	Paxs	474.50	Joback Method
dvisc	0.0001418	Paxs	510.46	Joback Method
dvisc	0.0001137	Paxs	546.42	Joback Method
dvisc	0.0000937	Paxs	582.38	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C75921685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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