

(3-Methoxyphenyl) methanol, isopropyl ether

Inchi:	InChI=1S/C11H16O2/c1-9(2)13-8-10-5-4-6-11(7-10)12-3/h4-7,9H,8H2,1-3H3
InchiKey:	DUXXMMBVXTVISE-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	COC1CCCC(COC(C)C)c1
Mol. weight [g/mol]:	180.24

Physical Properties

Property code	Value	Unit	Source
gf	-67.92	kJ/mol	Joback Method
hf	-315.03	kJ/mol	Joback Method
hfus	16.75	kJ/mol	Joback Method
hvap	47.45	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.620		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1357.00		NIST Webbook
rinpol	1357.00		NIST Webbook
tb	527.14	K	Joback Method
tc	731.36	K	Joback Method
tf	282.13	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.61	J/mol×K	527.14	Joback Method
cpg	366.95	J/mol×K	561.18	Joback Method
cpg	381.59	J/mol×K	595.21	Joback Method
cpg	395.53	J/mol×K	629.25	Joback Method
cpg	408.78	J/mol×K	663.29	Joback Method
cpg	421.33	J/mol×K	697.32	Joback Method
cpg	433.19	J/mol×K	731.36	Joback Method
dvisc	0.0019797	Pa×s	282.13	Joback Method

dvisc	0.0009620	Pa×s	322.96	Joback Method
dvisc	0.0005497	Pa×s	363.80	Joback Method
dvisc	0.0003516	Pa×s	404.63	Joback Method
dvisc	0.0002442	Pa×s	445.47	Joback Method
dvisc	0.0001802	Pa×s	486.31	Joback Method
dvisc	0.0001395	Pa×s	527.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U374590&Units=SI

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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