

(3-Methylphenyl) methanol, isopropyl ether

Inchi:	InChI=1S/C11H16O/c1-9(2)12-8-11-6-4-5-10(3)7-11/h4-7,9H,8H2,1-3H3
InchiKey:	RUFKLMFJFLCEFE-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	Cc1cccc(COC(C)C)c1
Mol. weight [g/mol]:	164.24

Physical Properties

Property code	Value	Unit	Source
gf	37.08	kJ/mol	Joback Method
hf	-182.81	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	45.04	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.920		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1212.00		NIST Webbook
tb	504.72	K	Joback Method
tc	710.80	K	Joback Method
tf	259.90	K	Joback Method
vc	0.555	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.28	J/molxK	504.72	Joback Method
cpg	341.96	J/molxK	539.07	Joback Method
cpg	356.87	J/molxK	573.41	Joback Method
cpg	371.02	J/molxK	607.76	Joback Method
cpg	384.44	J/molxK	642.11	Joback Method
cpg	397.14	J/molxK	676.45	Joback Method
cpg	409.13	J/molxK	710.80	Joback Method
dvisc	0.0027032	Paxs	259.90	Joback Method
dvisc	0.0012429	Paxs	300.70	Joback Method

dvisc	0.0006880	Paxs	341.51	Joback Method
dvisc	0.0004321	Paxs	382.31	Joback Method
dvisc	0.0002969	Paxs	423.11	Joback Method
dvisc	0.0002179	Paxs	463.92	Joback Method
dvisc	0.0001681	Paxs	504.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374583&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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