

(3-Methoxyphenyl) methanol, 2-methylpropyl ether

Inchi:	InChI=1S/C12H18O2/c1-10(2)8-14-9-11-5-4-6-12(7-11)13-3/h4-7,10H,8-9H2,1-3H3
InchiKey:	AYQBDUGDCKAUBY-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	COc1cccc(COCC(C)C)c1
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
gf	-59.50	kJ/mol	Joback Method
hf	-335.67	kJ/mol	Joback Method
hfus	19.34	kJ/mol	Joback Method
hvap	49.68	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.868		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinsol	1450.00		NIST Webbook
tb	550.02	K	Joback Method
tc	751.26	K	Joback Method
tf	293.40	K	Joback Method
vc	0.629	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.86	J/molxK	550.02	Joback Method
cpg	472.18	J/molxK	717.72	Joback Method
cpg	459.00	J/molxK	684.18	Joback Method
cpg	445.09	J/molxK	650.64	Joback Method
cpg	430.43	J/molxK	617.10	Joback Method
cpg	415.03	J/molxK	583.56	Joback Method
cpg	484.61	J/molxK	751.26	Joback Method
dvisc	0.0001287	Paxs	550.02	Joback Method
dvisc	0.0001672	Paxs	507.25	Joback Method

dvisc	0.0002278	Paxs	464.48	Joback Method
dvisc	0.0003305	Paxs	421.71	Joback Method
dvisc	0.0005216	Paxs	378.94	Joback Method
dvisc	0.0009244	Paxs	336.17	Joback Method
dvisc	0.0019359	Paxs	293.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374589&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
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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