

(3-Methoxyphenyl) methanol, 2-methylbutyl ether

Inchi:	InChI=1S/C13H20O2/c1-4-11(2)9-15-10-12-6-5-7-13(8-12)14-3/h5-8,11H,4,9-10H2,1-3H
InchiKey:	SZDSQJQEAAAYUTJ-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	CCC(C)COCc1cccc(OC)c1
Mol. weight [g/mol]:	208.30

Physical Properties

Property code	Value	Unit	Source
gf	-51.08	kJ/mol	Joback Method
hf	-356.31	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	51.90	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.258		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1556.00		NIST Webbook
tb	572.90	K	Joback Method
tc	771.30	K	Joback Method
tf	304.67	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.87	J/molxK	572.90	Joback Method
cpg	464.73	J/molxK	605.97	Joback Method
cpg	480.79	J/molxK	639.03	Joback Method
cpg	496.06	J/molxK	672.10	Joback Method
cpg	510.54	J/molxK	705.17	Joback Method
cpg	524.23	J/molxK	738.24	Joback Method
cpg	537.16	J/molxK	771.30	Joback Method
dvisc	0.0018691	Paxs	304.67	Joback Method
dvisc	0.0008781	Paxs	349.38	Joback Method

dvisc	0.0004897	Paxs	394.08	Joback Method
dvisc	0.0003076	Paxs	438.78	Joback Method
dvisc	0.0002105	Paxs	483.49	Joback Method
dvisc	0.0001537	Paxs	528.19	Joback Method
dvisc	0.0001178	Paxs	572.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374436&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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