

(2-Methylphenyl) methanol, 3-methylbutyl ether

Inchi:	InChI=1S/C13H20O/c1-11(2)8-9-14-10-13-7-5-4-6-12(13)3/h4-7,11H,8-10H2,1-3H3
InchiKey:	QPMBWRXBBBFSJF-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	Cc1ccccc1COCCC(C)C
Mol. weight [g/mol]:	192.30

Physical Properties

Property code	Value	Unit	Source
gf	53.92	kJ/mol	Joback Method
hf	-224.09	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	49.49	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.558		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1419.00		NIST Webbook
tb	550.48	K	Joback Method
tc	750.64	K	Joback Method
tf	282.44	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.77	J/molxK	550.48	Joback Method
cpg	438.01	J/molxK	583.84	Joback Method
cpg	454.39	J/molxK	617.20	Joback Method
cpg	469.93	J/molxK	650.56	Joback Method
cpg	484.66	J/molxK	683.92	Joback Method
cpg	498.59	J/molxK	717.28	Joback Method
cpg	511.75	J/molxK	750.64	Joback Method
dvisc	0.0026219	Paxs	282.44	Joback Method
dvisc	0.0011656	Paxs	327.11	Joback Method

dvisc	0.0006296	Paxs	371.79	Joback Method
dvisc	0.0003881	Paxs	416.46	Joback Method
dvisc	0.0002628	Paxs	461.13	Joback Method
dvisc	0.0001906	Paxs	505.81	Joback Method
dvisc	0.0001457	Paxs	550.48	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=U374709&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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