(4-Methylphenyl) methanol, 3-methylbutyl ether

Inchi: InChI=1S/C13H20O/c1-11(2)8-9-14-10-13-6-4-12(3)5-7-13/h4-7,11H,8-10H2,1-3H3
InchiKey: XPKWKRIVFZNOLI-UHFFFAOYSA-N
Formula: C13H20O
SMILES: Cc1ccc(COCCC(C)C)cc1
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	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
tb	550.48	K	Joback Method
tc	750.64	K	Joback Method
tf	282.44	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.77	J/mol×K	550.48	Joback Method
cpg	498.59	J/mol×K	717.28	Joback Method
cpg	484.66	J/mol×K	683.92	Joback Method
cpg	469.93	J/mol×K	650.56	Joback Method
cpg	454.39	J/mol×K	617.20	Joback Method
cpg	438.01	J/mol×K	583.84	Joback Method
cpg	511.75	J/mol×K	750.64	Joback Method
dvisc	0.0001457	Pa×s	550.48	Joback Method

dvisc	0.0001906	Pa×s	505.81	Joback Method
dvisc	0.0002628	Pa×s	461.13	Joback Method
dvisc	0.0003881	Pa×s	416.46	Joback Method
dvisc	0.0006296	Pa×s	371.79	Joback Method
dvisc	0.0011656	Pa×s	327.11	Joback Method
dvisc	0.0026219	Pa×s	282.44	Joback Method

Sources

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=U374657&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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