(3-Methylphenyl) methanol, neopentyl ether

Inchi: InChI=1S/C13H20O/c1-11-6-5-7-12(8-11)9-14-10-13(2,3)4/h5-8H,9-10H2,1-4H3
InchiKey: AGBLWVRAXHXNJN-UHFFFAOYSA-N
Formula: C13H20O
SMILES: Cc1cccc(COCC(C)(C)C)c1
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	59.20	kJ/mol	Joback Method
hf	-227.56	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	48.58	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.558		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1325.00		NIST Webbook
tb	547.69	K	Joback Method
tc	755.69	K	Joback Method
tf	299.86	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.50	J/mol×K	547.69	Joback Method
cpg	441.42	J/mol×K	582.36	Joback Method
cpg	458.32	J/mol×K	617.02	Joback Method
cpg	474.24	J/mol×K	651.69	Joback Method
cpg	489.20	J/mol×K	686.36	Joback Method
cpg	503.27	J/mol×K	721.02	Joback Method
cpg	516.46	J/mol×K	755.69	Joback Method
dvisc	0.0024476	Pa×s	299.86	Joback Method
dvisc	0.0011461	Pa×s	341.17	Joback Method

dvisc	0.0006322	Pa×s	382.47	Joback Method
dvisc	0.0003916	Pa×s	423.78	Joback Method
dvisc	0.0002641	Pa×s	465.08	Joback Method
dvisc	0.0001900	Pa×s	506.39	Joback Method
dvisc	0.0001436	Pa×s	547.69	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=U374441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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