

(3-Methylphenyl) methanol, n-butyl ether

Inchi: InChI=1S/C12H18O/c1-3-4-8-13-10-12-7-5-6-11(2)9-12/h5-7,9H,3-4,8,10H2,1-2H3
InchiKey: LZLXCRULGUUVAY-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CCCCOCCc1cccc(C)c1
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	47.94	kJ/mol	Joback Method
hf	-198.17	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	47.65	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.312		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	528.04	K	Joback Method
tc	726.82	K	Joback Method
tf	286.17	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.37	J/mol×K	528.04	Joback Method
cpg	445.32	J/mol×K	693.69	Joback Method
cpg	432.20	J/mol×K	660.56	Joback Method
cpg	418.37	J/mol×K	627.43	Joback Method
cpg	403.80	J/mol×K	594.30	Joback Method
cpg	388.47	J/mol×K	561.17	Joback Method
cpg	457.72	J/mol×K	726.82	Joback Method
dvisc	0.0001670	Pa×s	528.04	Joback Method

dvisc	0.0002127	Pa×s	487.73	Joback Method
dvisc	0.0002829	Pa×s	447.42	Joback Method
dvisc	0.0003982	Pa×s	407.11	Joback Method
dvisc	0.0006042	Pa×s	366.79	Joback Method
dvisc	0.0010163	Pa×s	326.48	Joback Method
dvisc	0.0019790	Pa×s	286.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U374442&Units=SI

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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