(2-Methylphenyl) methanol, 1-methylpropyl ether

Inchi: InChI=1S/C12H18O/c1-4-11(3)13-9-12-8-6-5-7-10(12)2/h5-8,11H,4,9H2,1-3H3
InchiKey: VUOKHHXUOHZBSA-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CCC(C)OCc1ccccc1C
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	45.50	kJ/mol	Joback Method
hf	-203.45	kJ/mol	Joback Method
hfus	18.15	kJ/mol	Joback Method
hvap	47.27	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.310		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1314.00		NIST Webbook
rinpol	1314.00		NIST Webbook
tb	527.60	K	Joback Method
tc	730.68	K	Joback Method
tf	271.17	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.63	J/mol×K	527.60	Joback Method
cpg	389.15	J/mol×K	561.45	Joback Method
cpg	404.85	J/mol×K	595.29	Joback Method
cpg	419.75	J/mol×K	629.14	Joback Method
cpg	433.88	J/mol×K	662.99	Joback Method
cpg	447.24	J/mol×K	696.83	Joback Method
cpg	459.86	J/mol×K	730.68	Joback Method
dvisc	0.0026822	Pa×s	271.17	Joback Method

dvisc	0.0012118	Pa×s	313.91	Joback Method
dvisc	0.0006624	Pa×s	356.65	Joback Method
dvisc	0.0004120	Pa×s	399.38	Joback Method
dvisc	0.0002809	Pa×s	442.12	Joback Method
dvisc	0.0002049	Pa×s	484.86	Joback Method
dvisc	0.0001573	Pa×s	527.60	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=U374443&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