2-Methoxybenzyl alcohol, neopentyl ether

Inchi: InChI=1S/C13H20O2/c1-13(2,3)10-15-9-11-7-5-6-8-12(11)14-4/h5-8H,9-10H2,1-4H3
InchiKey: TUBPCWPOXXWECY-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: COc1ccccc1COCC(C)(C)C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-45.80	kJ/mol	Joback Method
hf	-359.78	kJ/mol	Joback Method
hfus	18.04	kJ/mol	Joback Method
hvap	50.99	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.258		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
tb	570.11	K	Joback Method
tc	776.01	K	Joback Method
tf	322.09	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.60	J/mol×K	570.11	Joback Method
cpg	468.05	J/mol×K	604.43	Joback Method
cpg	484.54	J/mol×K	638.74	Joback Method
cpg	500.11	J/mol×K	673.06	Joback Method
cpg	514.78	J/mol×K	707.38	Joback Method
cpg	528.57	J/mol×K	741.69	Joback Method
cpg	541.51	J/mol×K	776.01	Joback Method
dvisc	0.0017084	Pa×s	322.09	Joback Method

dvisc	0.0008426	Pa×s	363.43	Joback Method
dvisc	0.0004802	Pa×s	404.76	Joback Method
dvisc	0.0003037	Pa×s	446.10	Joback Method
dvisc	0.0002076	Pa×s	487.44	Joback Method
dvisc	0.0001506	Pa×s	528.77	Joback Method
dvisc	0.0001144	Pa×s	570.11	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=U378199&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