

(3-Methoxyphenyl) methanol, neopentyl ether

Inchi:	InChI=1S/C13H20O2/c1-13(2,3)10-15-9-11-6-5-7-12(8-11)14-4/h5-8H,9-10H2,1-4H3
InchiKey:	DUTABBVANHOEMW-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	COc1cccc(COCC(C)(C)C)c1
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	1472.00		NIST Webbook
tb	570.11	K	Joback Method
tc	776.01	K	Joback Method
tf	322.09	K	Joback Method
vc	0.680	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.60	J/molxK	570.11	Joback Method
cpg	468.05	J/molxK	604.43	Joback Method
cpg	484.54	J/molxK	638.74	Joback Method
cpg	500.11	J/molxK	673.06	Joback Method
cpg	514.78	J/molxK	707.38	Joback Method
cpg	528.57	J/molxK	741.69	Joback Method
cpg	541.51	J/molxK	776.01	Joback Method
dvisc	0.0017084	Paxs	322.09	Joback Method
dvisc	0.0008426	Paxs	363.43	Joback Method

dvisc	0.0004802	Paxs	404.76	Joback Method
dvisc	0.0003037	Paxs	446.10	Joback Method
dvisc	0.0002076	Paxs	487.44	Joback Method
dvisc	0.0001506	Paxs	528.77	Joback Method
dvisc	0.0001144	Paxs	570.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U374595&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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