

(3-Methoxyphenyl) methanol, n-pentyl ether

Inchi:	InChI=1S/C13H20O2/c1-3-4-5-9-15-11-12-7-6-8-13(10-12)14-2/h6-8,10H,3-5,9,11H2,1-2
InchiKey:	SOMSDAGIKQRSQA-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	CCCCCOCc1ccc(OC)c1
Mol. weight [g/mol]:	208.30

Physical Properties

Property code	Value	Unit	Source
gf	-48.64	kJ/mol	Joback Method
hf	-351.03	kJ/mol	Joback Method
hfus	25.45	kJ/mol	Joback Method
hvap	52.29	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.402		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1600.00		NIST Webbook
tb	573.34	K	Joback Method
tc	767.84	K	Joback Method
tf	319.67	K	Joback Method
vc	0.692	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.53	J/molxK	573.34	Joback Method
cpg	522.36	J/molxK	735.43	Joback Method
cpg	508.89	J/molxK	703.01	Joback Method
cpg	494.68	J/molxK	670.59	Joback Method
cpg	479.72	J/molxK	638.17	Joback Method
cpg	464.01	J/molxK	605.76	Joback Method
cpg	535.09	J/molxK	767.84	Joback Method
dvisc	0.0001258	Paxs	573.34	Joback Method
dvisc	0.0001607	Paxs	531.06	Joback Method

dvisc	0.0002140	Paxs	488.78	Joback Method
dvisc	0.0003010	Paxs	446.50	Joback Method
dvisc	0.0004547	Paxs	404.23	Joback Method
dvisc	0.0007563	Paxs	361.95	Joback Method
dvisc	0.0014392	Paxs	319.67	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=U374594&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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