

(2-Methylphenyl) methanol, n-pentyl ether

Inchi:	InChI=1S/C13H20O/c1-3-4-7-10-14-11-13-9-6-5-8-12(13)2/h5-6,8-9H,3-4,7,10-11H2,1-2H
InchiKey:	RUHDECNSEVJLKK-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	CCCCCOCC1CCCC1C
Mol. weight [g/mol]:	192.30

Physical Properties

Property code	Value	Unit	Source
gf	56.36	kJ/mol	Joback Method
hf	-218.81	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.702		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1461.00		NIST Webbook
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tb	550.92	K	Joback Method
tc	747.00	K	Joback Method
tf	297.44	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.48	J/mol×K	550.92	Joback Method
cpg	437.30	J/mol×K	583.60	Joback Method
cpg	453.31	J/mol×K	616.28	Joback Method
cpg	468.53	J/mol×K	648.96	Joback Method
cpg	482.97	J/mol×K	681.64	Joback Method
cpg	496.65	J/mol×K	714.32	Joback Method
cpg	509.60	J/mol×K	747.00	Joback Method
dvisc	0.0019570	Pa×s	297.44	Joback Method

dvisc	0.0009863	Pa×s	339.69	Joback Method
dvisc	0.0005784	Pa×s	381.93	Joback Method
dvisc	0.0003773	Pa×s	424.18	Joback Method
dvisc	0.0002659	Pa×s	466.43	Joback Method
dvisc	0.0001986	Pa×s	508.67	Joback Method
dvisc	0.0001551	Pa×s	550.92	Joback Method

Sources

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=U374707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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