

(4-Methylphenyl) methanol, n-pentyl ether

Inchi:	InChI=1S/C13H20O/c1-3-4-5-10-14-11-13-8-6-12(2)7-9-13/h6-9H,3-5,10-11H2,1-2H3
InchiKey:	VYWRZFKFKKOLU-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	CCCCCOCc1ccc(C)cc1
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	1464.00		NIST Webbook
rinpol	1464.00		NIST Webbook
tb	550.92	K	Joback Method
tc	747.00	K	Joback Method
tf	297.44	K	Joback Method
vc	0.673	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.48	J/molxK	550.92	Joback Method
cpg	496.65	J/molxK	714.32	Joback Method
cpg	482.97	J/molxK	681.64	Joback Method
cpg	468.53	J/molxK	648.96	Joback Method
cpg	453.31	J/molxK	616.28	Joback Method
cpg	437.30	J/molxK	583.60	Joback Method
cpg	509.60	J/molxK	747.00	Joback Method
dvisc	0.0001551	Paxs	550.92	Joback Method

dvisc	0.0001986	Paxs	508.67	Joback Method
dvisc	0.0002659	Paxs	466.43	Joback Method
dvisc	0.0003773	Paxs	424.18	Joback Method
dvisc	0.0005784	Paxs	381.93	Joback Method
dvisc	0.0009863	Paxs	339.69	Joback Method
dvisc	0.0019570	Paxs	297.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374658&Units=SI
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

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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