

2-Methyl-1-phenyl-1-pentanol

Inchi:	InChI=1S/C12H18O/c1-3-7-10(2)12(13)11-8-5-4-6-9-11/h4-6,8-10,12-13H,3,7H2,1-2H3
InchiKey:	AKMRXUUGAJOMFO-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CCCC(C)C(O)c1ccccc1
Mol. weight [g/mol]:	178.27
CAS:	73177-67-0

Physical Properties

Property code	Value	Unit	Source
gf	20.87	kJ/mol	Joback Method
hf	-217.27	kJ/mol	Joback Method
hfus	17.92	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.156		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
tb	591.94	K	Joback Method
tc	787.01	K	Joback Method
tf	282.24	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.68	J/molxK	591.94	Joback Method
cpg	422.21	J/molxK	624.45	Joback Method
cpg	435.93	J/molxK	656.96	Joback Method
cpg	448.87	J/molxK	689.48	Joback Method
cpg	461.06	J/molxK	721.99	Joback Method
cpg	472.53	J/molxK	754.50	Joback Method
cpg	483.32	J/molxK	787.01	Joback Method
dvisc	0.0286301	Paxs	282.24	Joback Method
dvisc	0.0047767	Paxs	333.86	Joback Method

dvisc	0.0012874	Paxs	385.47	Joback Method
dvisc	0.0004729	Paxs	437.09	Joback Method
dvisc	0.0002146	Paxs	488.71	Joback Method
dvisc	0.0001133	Paxs	540.32	Joback Method
dvisc	0.0000668	Paxs	591.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C73177670&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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