

4-Methyl-4-phenyl-2-pentanol

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

Physical Properties

Property code	Value	Unit	Source
gf	26.15	kJ/mol	Joback Method
hf	-220.74	kJ/mol	Joback Method
hfus	14.03	kJ/mol	Joback Method
hvap	59.58	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.735		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
tb	589.15	K	Joback Method
tc	791.28	K	Joback Method
tf	299.66	K	Joback Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.54	J/mol×K	589.15	Joback Method
cpg	425.50	J/mol×K	622.84	Joback Method
cpg	439.51	J/mol×K	656.53	Joback Method
cpg	452.62	J/mol×K	690.22	Joback Method
cpg	464.88	J/mol×K	723.90	Joback Method
cpg	476.36	J/mol×K	757.59	Joback Method
cpg	487.10	J/mol×K	791.28	Joback Method
dvisc	0.0192526	Paxs	299.66	Joback Method
dvisc	0.0038611	Paxs	347.91	Joback Method
dvisc	0.0011452	Paxs	396.16	Joback Method

dvisc	0.0004423	Paxs	444.40	Joback Method
dvisc	0.0002058	Paxs	492.65	Joback Method
dvisc	0.0001098	Paxs	540.90	Joback Method
dvisc	0.0000649	Paxs	589.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004202&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
hvac:	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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