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	m3/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	Pa×s	299.66	Joback Method
dvisc	0.0038611	Pa×s	347.91	Joback Method
dvisc	0.0011452	Pa×s	396.16	Joback Method

dvisc	0.0004423	Pa×s	444.40	Joback Method
dvisc	0.0002058	Pa×s	492.65	Joback Method
dvisc	0.0001098	Pa×s	540.90	Joback Method
dvisc	0.0000649	Pa×s	589.15	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=B6004202&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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