

2-Phenyl-4-penten-2-ol

Inchi:	InChI=1S/C11H14O/c1-3-9-11(2,12)10-7-5-4-6-8-10/h3-8,12H,1,9H2,2H3
InchiKey:	BELRNEPYFJNSPN-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	C=CCC(C)(O)c1ccccc1
Mol. weight [g/mol]:	162.23
CAS:	61077-65-4

Physical Properties

Property code	Value	Unit	Source
gf	108.01	kJ/mol	Joback Method
hf	-69.39	kJ/mol	Joback Method
hfus	13.68	kJ/mol	Joback Method
hvap	57.07	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.470		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	563.39	K	Joback Method
tc	768.43	K	Joback Method
tf	301.63	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.97	J/mol×K	563.39	Joback Method
cpg	355.37	J/mol×K	597.56	Joback Method
cpg	367.85	J/mol×K	631.74	Joback Method
cpg	379.47	J/mol×K	665.91	Joback Method
cpg	390.29	J/mol×K	700.08	Joback Method
cpg	400.37	J/mol×K	734.26	Joback Method
cpg	409.77	J/mol×K	768.43	Joback Method
dvisc	0.0135190	Pa×s	301.63	Joback Method
dvisc	0.0034291	Pa×s	345.26	Joback Method

dvisc	0.0011833	Pa×s	388.88	Joback Method
dvisc	0.0005061	Pa×s	432.51	Joback Method
dvisc	0.0002529	Pa×s	476.14	Joback Method
dvisc	0.0001420	Pa×s	519.76	Joback Method
dvisc	0.0000872	Pa×s	563.39	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=C61077654&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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