

Alpha-phenyl-o-toluic acid

Other names:	o-benzylbenzoic acid
Inchi:	InChI=1S/C14H12O2/c15-14(16)13-9-5-4-8-12(13)10-11-6-2-1-3-7-11/h1-9H,10H2,(H,15
InchiKey:	FESDHLVLVYZNFY-UHFFFAOYSA-N
Formula:	C14H12O2
SMILES:	O=C(O)c1cccc1Cc1cccc1
Mol. weight [g/mol]:	212.24
CAS:	612-35-1

Physical Properties

Property code	Value	Unit	Source
gf	16.45	kJ/mol	Joback Method
hf	-135.51	kJ/mol	Joback Method
hfus	25.40	kJ/mol	Joback Method
hvap	75.40	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.976		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	724.11	K	Joback Method
tc	950.68	K	Joback Method
tf	423.65	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.76	J/mol×K	724.11	Joback Method
cpg	491.94	J/mol×K	912.92	Joback Method
cpg	483.34	J/mol×K	875.16	Joback Method
cpg	473.98	J/mol×K	837.40	Joback Method
cpg	463.80	J/mol×K	799.63	Joback Method
cpg	452.75	J/mol×K	761.87	Joback Method
cpg	499.84	J/mol×K	950.68	Joback Method
dvisc	0.0000433	Pa×s	724.11	Joback Method

dvisc	0.0000627	Pa×s	674.03	Joback Method
dvisc	0.0000964	Pa×s	623.96	Joback Method
dvisc	0.0001598	Pa×s	573.88	Joback Method
dvisc	0.0002916	Pa×s	523.80	Joback Method
dvisc	0.0006041	Pa×s	473.73	Joback Method
dvisc	0.0014870	Pa×s	423.65	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=C612351&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
mccvol:	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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