

Benzoic acid, 4-(phenylmethyl)-

Other names:	4-(Phenylmethyl)benzoic acid
Inchi:	InChI=1S/C14H12O2/c15-14(16)13-8-6-12(7-9-13)10-11-4-2-1-3-5-11/h1-9H,10H2,(H,15
InchiKey:	FPHVRPCVNPBPBH-UHFFFAOYSA-N
Formula:	C14H12O2
SMILES:	O=C(O)c1ccc(Cc2ccccc2)cc1
Mol. weight [g/mol]:	212.24
CAS:	620-86-0

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.76	J/molxK	724.11	Joback Method
cpg	452.75	J/molxK	761.87	Joback Method
cpg	463.80	J/molxK	799.63	Joback Method
cpg	473.98	J/molxK	837.40	Joback Method
cpg	483.34	J/molxK	875.16	Joback Method
cpg	491.94	J/molxK	912.92	Joback Method
cpg	499.84	J/molxK	950.68	Joback Method
dvisc	0.0014870	Paxs	423.65	Joback Method

dvisc	0.0006041	Paxs	473.73	Joback Method
dvisc	0.0002916	Paxs	523.80	Joback Method
dvisc	0.0001598	Paxs	573.88	Joback Method
dvisc	0.0000964	Paxs	623.96	Joback Method
dvisc	0.0000627	Paxs	674.03	Joback Method
dvisc	0.0000433	Paxs	724.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620860&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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