

p-Cyclohexylbenzoic acid

Other names:	4-Cyclohexylbenzoic acid Benzoic acid, 4-cyclohexyl-
Inchi:	InChI=1S/C13H16O2/c14-13(15)12-8-6-11(7-9-12)10-4-2-1-3-5-10/h6-10H,1-5H2,(H,14,15)
InchiKey:	QCIWHVKGVVQHIY-UHFFFAOYSA-N
Formula:	C13H16O2
SMILES:	O=C(O)c1ccc(C2CCCCC2)cc1
Mol. weight [g/mol]:	204.26
CAS:	20029-52-1

Physical Properties

Property code	Value	Unit	Source
gf	-79.93	kJ/mol	Joback Method
hf	-297.08	kJ/mol	Joback Method
hfus	20.60	kJ/mol	Joback Method
hvap	71.32	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.433		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	694.10	K	Joback Method
tc	918.25	K	Joback Method
tf	393.34	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.22	J/mol×K	694.10	Joback Method
cpg	481.49	J/mol×K	731.46	Joback Method
cpg	495.64	J/mol×K	768.82	Joback Method
cpg	508.72	J/mol×K	806.17	Joback Method
cpg	520.77	J/mol×K	843.53	Joback Method
cpg	531.85	J/mol×K	880.89	Joback Method
cpg	542.00	J/mol×K	918.25	Joback Method

dvisc	0.0028999	Pa×s	393.34	Joback Method
dvisc	0.0010286	Pa×s	443.47	Joback Method
dvisc	0.0004504	Pa×s	493.59	Joback Method
dvisc	0.0002296	Pa×s	543.72	Joback Method
dvisc	0.0001312	Pa×s	593.85	Joback Method
dvisc	0.0000818	Pa×s	643.97	Joback Method
dvisc	0.0000546	Pa×s	694.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20029521&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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