4-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,14,1
InchiKey: QCIWHVKGVVQHIY-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: O=C(O)c1ccc(C2CCCCC2)cc1
Mol. weight [g/mol]: 204.27

Physical Properties

Property code	Value	Unit	Source
af	0.7219		Cheméo Relay (1.0)
gf	-79.93	kJ/mol	Joback Method
hf	-390.88	kJ/mol	Cheméo Relay (1.0)
hfus	20.60	kJ/mol	Joback Method
hvap	103.09	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-4.01		Cheméo Relay (1.0)
logp	3.433		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	610.51	K	Cheméo Relay (1.0)
tc	859.19	K	Cheméo Relay (1.0)
tf	476.90	K	Cheméo Relay (1.0)
vc	0.577	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	481.49	J/mol×K	731.46	Joback Method
dvisc	0.0002296	Pa×s	543.72	Joback Method
dvisc	0.0000546	Pa×s	694.10	Joback Method
dvisc	0.0000818	Pa×s	643.97	Joback Method
dvisc	0.0001312	Pa×s	593.85	Joback Method
dvisc	0.0028999	Pa×s	393.34	Joback Method
dvisc	0.0004504	Pa×s	493.59	Joback Method
dvisc	0.0010286	Pa×s	443.47	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20029521&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
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