Cyclohexanecarboxylic acid, 1-cyclohexyl-

Other names: [1,1'-bicyclohexyl]-1-carboxylic acid
Inchi: InChI=1S/C13H22O2/c14-12(15)13(9-5-2-6-10-13)11-7-3-1-4-8-11/h11H,1-10H2,(H,14,1
InchiKey: SJSRFXJWBKOROD-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: O=C(O)C1(C2CCCCC2)CCCCC1
Mol. weight [g/mol]: 210.31
CAS: 60263-54-9

Physical Properties

Property code	Value	Unit	Source
gf	-163.75	kJ/mol	Joback Method
hf	-452.58	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	67.66	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.602		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
tb	682.23	K	Joback Method
tc	906.87	K	Joback Method
tf	385.68	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.21	J/mol×K	682.23	Joback Method
cpg	556.42	J/mol×K	719.67	Joback Method
cpg	574.53	J/mol×K	757.11	Joback Method
cpg	591.67	J/mol×K	794.55	Joback Method
cpg	608.01	J/mol×K	831.99	Joback Method
cpg	623.68	J/mol×K	869.43	Joback Method
cpg	638.82	J/mol×K	906.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60263549&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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