1,1-Cyclobutanedicarboxylic acid

Other names: Cyclobutane-1,1-dicarboxylic acid
Inchi: InChI=1S/C6H8O4/c7-4(8)6(5(9)10)2-1-3-6/h1-3H2,(H,7,8)(H,9,10)
InchiKey: CCQPAEQGAVNNIA-UHFFFAOYSA-N
Formula: C6H8O4
SMILES: O=C(O)C1(C(=O)O)CCC1
Mol. weight [g/mol]: 144.13
CAS: 5445-51-2

Physical Properties

Property code	Value	Unit	Source
gf	-488.68	kJ/mol	Joback Method
hf	-724.50 ± 1.20	kJ/mol	NIST Webbook
hfs	-835.70 ± 1.00	kJ/mol	NIST Webbook
hfus	12.41	kJ/mol	Joback Method
hsub	111.20	kJ/mol	NIST Webbook
hsub	111.20 ± 0.70	kJ/mol	NIST Webbook
hvap	74.73	kJ/mol	Joback Method
log10ws	-0.19		Crippen Method
logp	0.326		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	6065.55	kPa	Joback Method
tb	640.03	K	Joback Method
tc	834.91	K	Joback Method
tf	417.20	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.17	J/mol×K	640.03	Joback Method
cpg	266.26	J/mol×K	672.51	Joback Method
cpg	273.01	J/mol×K	704.99	Joback Method
cpg	279.49	J/mol×K	737.47	Joback Method
cpg	285.80	J/mol×K	769.95	Joback Method

cpg	292.02	J/mol×K	802.43	Joback Method
cpg	298.24	J/mol×K	834.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5445512&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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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

Latest version available from:
https://www.chemeo.com/cid/63-246-9/1-1-Cyclobutanedicarboxylic-acid.pdf
Generated by Cheméo on 2024-05-01 11:24:15.730180994 +0000 UTC m=+16851904.650758314.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.