

Cyclopentanecarboxylic acid

Inchi:	InChI=1S/C8H15NO2/c1-2-11-7(10)8(9)5-3-4-6-8/h2-6,9H2,1H3
InchiKey:	NLLGKNYQDQBMFW-UHFFFAOYSA-N
Formula:	C8H15NO2
SMILES:	CCOC(=O)C1(N)CCCC1
Mol. weight [g/mol]:	157.21
CAS:	1664-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-119.93	kJ/mol	Joback Method
hf	-343.74	kJ/mol	Joback Method
hfus	12.10	kJ/mol	Joback Method
hvap	52.31	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	0.821		Crippen Method
mcvol	130.140	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	1070.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1045.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
tb	546.78	K	Joback Method
tc	769.68	K	Joback Method
tf	370.14	K	Joback Method
vc	0.475	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.48	J/mol×K	546.78	Joback Method

cpg	338.26	J/mol×K	583.93	Joback Method
cpg	352.11	J/mol×K	621.08	Joback Method
cpg	365.13	J/mol×K	658.23	Joback Method
cpg	377.44	J/mol×K	695.38	Joback Method
cpg	389.15	J/mol×K	732.53	Joback Method
cpg	400.39	J/mol×K	769.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1664353&Units=SI
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

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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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