

1,3-Cyclopentanedicarboximide

Inchi:	InChI=1S/C7H9NO2/c9-6-4-1-2-5(3-4)7(10)8-6/h4-5H,1-3H2,(H,8,9,10)
InchiKey:	CXCNSNHPXLOUNF-UHFFFAOYSA-N
Formula:	C7H9NO2
SMILES:	O=C1NC(=O)C2CCC1C2
Mol. weight [g/mol]:	139.15
CAS:	5763-45-1

Physical Properties

Property code	Value	Unit	Source
gf	-52.11	kJ/mol	Joback Method
hf	-292.12	kJ/mol	Joback Method
hfus	14.57	kJ/mol	Joback Method
hvap	46.60	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.059		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	565.77	K	Joback Method
tc	821.83	K	Joback Method
tf	438.96	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.21	J/molxK	565.77	Joback Method
cpg	272.94	J/molxK	608.45	Joback Method
cpg	287.78	J/molxK	651.12	Joback Method
cpg	301.71	J/molxK	693.80	Joback Method
cpg	314.71	J/molxK	736.48	Joback Method
cpg	326.75	J/molxK	779.15	Joback Method
cpg	337.82	J/molxK	821.83	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5763451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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