1,4-Cyclooctanedione

Inchi: InChI=1S/C8H12O2/c9-7-3-1-2-4-8(10)6-5-7/h1-6H2
InchiKey: LZTHLBQVLFQNKK-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: O=C1CCCCC(=O)CC1
Mol. weight [g/mol]: 140.18
CAS: 55794-45-1

Physical Properties

Property code	Value	Unit	Source
gf	-220.74	kJ/mol	Joback Method
hf	-421.51	kJ/mol	Joback Method
hfus	2.06	kJ/mol	Joback Method
hvap	42.98	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.479		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	550.84	K	Joback Method
tc	806.42	K	Joback Method
tf	320.94	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.89	J/mol×K	550.84	Joback Method
cpg	294.34	J/mol×K	593.44	Joback Method
cpg	311.86	J/mol×K	636.03	Joback Method
cpg	328.36	J/mol×K	678.63	Joback Method
cpg	343.76	J/mol×K	721.23	Joback Method
cpg	358.00	J/mol×K	763.82	Joback Method
cpg	371.00	J/mol×K	806.42	Joback Method
hfust	11.92	kJ/mol	341.20	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55794451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
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