1,3-Cyclohexanedione, 4-propyl-

Inchi: InChI=1S/C9H14O2/c1-2-3-7-4-5-8(10)6-9(7)11/h7H,2-6H2,1H3
InchiKey: WWLVJBISOZBFCG-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CCCC1CCC(=O)CC1=O
Mol. weight [g/mol]: 154.21
CAS: 18456-81-0

Physical Properties

Property code	Value	Unit	Source
gf	-195.83	kJ/mol	Joback Method
hf	-450.17	kJ/mol	Joback Method
hfus	9.92	kJ/mol	Joback Method
hvap	44.55	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.725		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	560.51	K	Joback Method
tc	792.97	K	Joback Method
tf	335.01	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.42	J/mol×K	560.51	Joback Method
cpg	341.03	J/mol×K	599.25	Joback Method
cpg	357.81	J/mol×K	638.00	Joback Method
cpg	373.72	J/mol×K	676.74	Joback Method
cpg	388.73	J/mol×K	715.48	Joback Method
cpg	402.78	J/mol×K	754.23	Joback Method
cpg	415.83	J/mol×K	792.97	Joback Method

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=C18456810&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
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