1,3-Cyclopentanedione, 4-butyl-

Other names: 4-Butyl-1,3-cyclopentanedione
Inchi: InChI=1S/C9H14O2/c1-2-3-4-7-5-8(10)6-9(7)11/h7H,2-6H2,1H3
InchiKey: UDVQUWZQMOBAGE-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CCCCC1CC(=O)CC1=O
Mol. weight [g/mol]: 154.21
CAS: 54244-72-3

Physical Properties

Property code	Value	Unit	Source
gf	-183.73	kJ/mol	Joback Method
hf	-444.01	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	44.38	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.725		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1129.00		NIST Webbook
tb	556.24	K	Joback Method
tc	780.50	K	Joback Method
tf	338.53	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.68	J/mol×K	556.24	Joback Method
cpg	339.24	J/mol×K	593.62	Joback Method
cpg	355.05	J/mol×K	630.99	Joback Method
cpg	370.10	J/mol×K	668.37	Joback Method
cpg	384.34	J/mol×K	705.75	Joback Method
cpg	397.75	J/mol×K	743.12	Joback Method
cpg	410.30	J/mol×K	780.50	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=C54244723&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume