1,3-Cyclobutanedione, 2,4-diethyl-2,4-dimethyl-

Inchi: InChI=1S/C10H16O2/c1-5-9(3)7(11)10(4,6-2)8(9)12/h5-6H2,1-4H3
InchiKey: XDYPAGRCWAXXGS-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CCC1(C)C(=O)C(C)(CC)C1=O
Mol. weight [g/mol]: 168.23
CAS: 7116-94-1

Physical Properties

Property code	Value	Unit	Source
gf	-181.90	kJ/mol	Joback Method
hf	-448.35	kJ/mol	Joback Method
hfus	5.19	kJ/mol	Joback Method
hvap	43.82	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.971		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	570.66	K	Joback Method
tc	801.02	K	Joback Method
tf	396.88	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.69	J/mol×K	570.66	Joback Method
cpg	384.95	J/mol×K	609.05	Joback Method
cpg	400.42	J/mol×K	647.45	Joback Method
cpg	415.28	J/mol×K	685.84	Joback Method
cpg	429.71	J/mol×K	724.24	Joback Method
cpg	443.87	J/mol×K	762.63	Joback Method
cpg	457.95	J/mol×K	801.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7116941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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