2-Cyclohexene-1-carboxylic acid, 2-methyl-4-oxo-, ethyl ester

Other names: Ethyl 2-methyl-4-oxo-2-cyclohexencarboxylate
Hagemann's ester
ethyl 2-methyl-4-oxocyclohex-2-enecarboxylate

Inchi: InChI=1S/C10H14O3/c1-3-13-10(12)9-5-4-8(11)6-7(9)2/h6,9H,3-5H2,1-2H3

InchiKey: VLTANIMRIRCCOQ-UHFFFAOYSA-N

Formula: C10H14O3

SMILES: CCOC(=O)C1CCC(=O)C=C1C

Mol. weight [g/mol]: 182.22

CAS: 487-51-4

Physical Properties

Property code	Value	Unit	Source
gf	-278.41	kJ/mol	Joback Method
hf	-531.60	kJ/mol	Joback Method
hfus	16.62	kJ/mol	Joback Method
hvap	52.64	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.475		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
tb	596.00	K	Joback Method
tc	818.34	K	Joback Method
tf	363.50	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.88	J/mol×K	596.00	Joback Method
cpg	383.76	J/mol×K	633.06	Joback Method
cpg	398.81	J/mol×K	670.11	Joback Method
cpg	413.02	J/mol×K	707.17	Joback Method
cpg	426.36	J/mol×K	744.23	Joback Method
cpg	438.80	J/mol×K	781.29	Joback Method

cpg	450.31	J/mol×K	818.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C487514&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