Cyclohexanecarboxylic acid, 2-oxo-, ethyl ester

Other names: Ethyl cyclohexanone-2-carboxylate
Ethyl 2-cyclohexanone-1-carboxylate
2-Carbethoxy cyclohexanone
Ethyl 2-oxocyclohexanecarboxylate
Cyclohexanone-2-carboxylic acid ethyl ester
Ethyl 2-cyclohexanonecarboxylate
Ethyl 1-oxo-2-cyclohexanecarboxylate
Ethyl 2-oxo-1-cyclohexanecarboxylate
Ethyl 2-oxocylohexanecarboxylate
Ethyl 2-oxylcyclohexanecarboxylic
2-(Ethoxycarbonyl)cyclohexanone
2-Cyclohexanonecarboxylic acid ethyl ester
2-Oxocyclohexanecarboxylic acid ethyl ester
NSC 18744

Inchi: InChI=1S/C9H14O3/c1-2-12-9(11)7-5-3-4-6-8(7)10/h7H,2-6H2,1H3

InchiKey: FGSGHBPKHFDJOP-UHFFFAOYSA-N

Formula: C9H14O3

SMILES: CCOC(=O)C1CCCCC1=O

Mol. weight [g/mol]: 170.21

CAS: 1655-07-8

Physical Properties

Property code	Value	Unit	Source
gf	-307.16	kJ/mol	Joback Method
hf	-557.27	kJ/mol	Joback Method
hfus	13.20	kJ/mol	Joback Method
hvap	49.46	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.309		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	568.98	K	Joback Method
tc	792.29	K	Joback Method
tf	338.95	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.68	J/mol×K	568.98	Joback Method
cpg	356.21	J/mol×K	606.20	Joback Method
cpg	371.90	J/mol×K	643.42	Joback Method
cpg	386.73	J/mol×K	680.63	Joback Method
cpg	400.67	J/mol×K	717.85	Joback Method
cpg	413.71	J/mol×K	755.07	Joback Method
cpg	425.83	J/mol×K	792.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.20	K	1.50	NIST Webbook

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=C1655078&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume