Cyclopentanecarboxylic acid, 2-oxo-, ethyl ester

Other names: «alpha»-(Carboethoxy)cyclopentanone
Ethyl cyclopentanone-2-carboxylate
Ethyl 2-cyclopentanone-1-carboxylate
Ethyl 2-cyclopentanonecarboxylate
Ethyl 2-oxo-1-cyclopentanecarboxylate
Ethyl 2-oxocyclopentanecarboxylate
Ethyl 2-oxoocyclopentanecarboxylate
2-(Ethoxycarbonyl)cyclopentanone
2-Carbethoxy-1-cyclopentanone
2-Carbethoxycyclopentanone
2-Cyclopentanonecarboxylic acid ethyl ester
Cyclopentanone-2-carboxylic acid ethyl ester
2-Carboethoxycyclopentanone
Ethyl ester of 2-oxocyclopentanecarboxylic acid
2-(Ethoxycarbonyl)-1-cyclopentanone

Inchi: InChI=1S/C8H12O3/c1-2-11-8(10)6-4-3-5-7(6)9/h6H,2-5H2,1H3

InchiKey: JHZPNBKZPAWCJD-UHFFFAOYSA-N

Formula: C8H12O3

SMILES: CCOC(=O)C1CCCC1=O

Mol. weight [g/mol]: 156.18

CAS: 611-10-9

Physical Properties

Property code	Value	Unit	Source
gf	-303.48	kJ/mol	Joback Method
hf	-530.47	kJ/mol	Joback Method
hfus	12.71	kJ/mol	Joback Method
hvap	47.06	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.919		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	541.83	K	Joback Method
tc	761.25	K	Joback Method
tf	331.20	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.08	J/mol×K	541.83	Joback Method
cpg	306.74	J/mol×K	578.40	Joback Method
cpg	320.71	J/mol×K	614.97	Joback Method
cpg	333.97	J/mol×K	651.54	Joback Method
cpg	346.52	J/mol×K	688.11	Joback Method
cpg	358.33	J/mol×K	724.68	Joback Method
cpg	369.38	J/mol×K	761.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	1.50	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C611109&Units=SI

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