Cyclohexanepropionic acid, 4-oxo-, ethyl ester

Other names: 3-(4-Oxocyclohexyl)-propionic acid, ethyl ester
Inchi: InChI=1S/C11H18O3/c1-2-14-11(13)8-5-9-3-6-10(12)7-4-9/h9H,2-8H2,1H3
InchiKey: IPJGROZEJICJSS-UHFFFAOYSA-N
Formula: C11H18O3
SMILES: CCOC(=O)CCC1CCC(=O)CC1
Mol. weight [g/mol]: 198.26
CAS: 58012-66-1

Physical Properties

Property code	Value	Unit	Source
gf	-290.32	kJ/mol	Joback Method
hf	-598.55	kJ/mol	Joback Method
hfus	18.38	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.089		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
tb	614.74	K	Joback Method
tc	830.21	K	Joback Method
tf	361.49	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.28	J/mol×K	614.74	Joback Method
cpg	457.15	J/mol×K	650.65	Joback Method
cpg	474.06	J/mol×K	686.56	Joback Method
cpg	489.98	J/mol×K	722.47	Joback Method
cpg	504.91	J/mol×K	758.39	Joback Method
cpg	518.83	J/mol×K	794.30	Joback Method
cpg	531.74	J/mol×K	830.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58012661&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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