1-Cycloheptene-1-carboxylic acid, 6-oxo-, methyl ester

Inchi: InChI=1S/C9H12O3/c1-12-9(11)7-4-2-3-5-8(10)6-7/h4H,2-3,5-6H2,1H3
InchiKey: OYDFMULXKLIRIL-UHFFFAOYSA-N
Formula: C9H12O3
SMILES: COC(=O)C1=CCCCC(=O)C1
Mol. weight [g/mol]: 168.19
CAS: 42205-56-1

Physical Properties

Property code	Value	Unit	Source
gf	-291.22	kJ/mol	Joback Method
hf	-496.78	kJ/mol	Joback Method
hfus	10.86	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.229		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	582.06	K	Joback Method
tc	816.73	K	Joback Method
tf	352.95	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.77	J/mol×K	582.06	Joback Method
cpg	334.33	J/mol×K	621.17	Joback Method
cpg	349.05	J/mol×K	660.28	Joback Method
cpg	362.88	J/mol×K	699.40	Joback Method
cpg	375.80	J/mol×K	738.51	Joback Method
cpg	387.76	J/mol×K	777.62	Joback Method
cpg	398.75	J/mol×K	816.73	Joback Method

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=C42205561&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume