Cyclohexanone--2-carboxylic acid, benzyl ester

Inchi: InChI=1S/C14H16O3/c15-13-9-5-4-8-12(13)14(16)17-10-11-6-2-1-3-7-11/h1-3,6-7,12H,4

InchiKey: UZOGMVJYLSQKCU-UHFFFAOYSA-N

Formula: C14H16O3

SMILES: O=C1CCCCC1C(=O)OCc1ccccc1

Mol. weight [g/mol]: 232.28

CAS: 2205-32-5

Physical Properties

Property code	Value	Unit	Source
gf	-152.65	kJ/mol	Joback Method
hf	-423.94	kJ/mol	Joback Method
hfus	20.19	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.489		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	710.06	K	Joback Method
tc	956.53	K	Joback Method
tf	421.72	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.18	J/mol×K	710.06	Joback Method
cpg	536.39	J/mol×K	751.14	Joback Method
cpg	553.11	J/mol×K	792.22	Joback Method
cpg	568.32	J/mol×K	833.29	Joback Method
cpg	582.04	J/mol×K	874.37	Joback Method
cpg	594.27	J/mol×K	915.45	Joback Method
cpg	605.03	J/mol×K	956.53	Joback Method

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=C2205325&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume