Cyclohexane-1-carboxylic acid, 1-methyl, methyl ester

Inchi: InChI=1S/C9H16O2/c1-9(8(10)11-2)6-4-3-5-7-9/h3-7H2,1-2H3
InchiKey: NKZISBBWNQEPAH-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: COC(=O)C1(C)CCCCC1
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-190.06	kJ/mol	Joback Method
hf	-404.33	kJ/mol	Joback Method
hfus	7.39	kJ/mol	Joback Method
hvap	44.06	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.130		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1026.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1026.00		NIST Webbook
tb	501.40	K	Joback Method
tc	718.78	K	Joback Method
tf	294.63	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.50	J/mol×K	501.40	Joback Method
cpg	325.53	J/mol×K	537.63	Joback Method
cpg	341.50	J/mol×K	573.86	Joback Method
cpg	356.52	J/mol×K	610.09	Joback Method
cpg	370.67	J/mol×K	646.32	Joback Method
cpg	384.06	J/mol×K	682.55	Joback Method
cpg	396.78	J/mol×K	718.78	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=R140&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume