Cyclohexanecarboxylic acid, 1-ethyl-, methyl ester

Other names: Methyl 1-ethyl-1-cyclohexanecarboxylate
Inchi: InChI=1S/C10H18O2/c1-3-10(9(11)12-2)7-5-4-6-8-10/h3-8H2,1-2H3
InchiKey: JPAPFFYGFBXJAK-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCC1(C(=O)OC)CCCCC1
Mol. weight [g/mol]: 170.25
CAS: 4630-81-3

Physical Properties

Property code	Value	Unit	Source
gf	-181.64	kJ/mol	Joback Method
hf	-424.97	kJ/mol	Joback Method
hfus	9.98	kJ/mol	Joback Method
hvap	46.29	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.520		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	1122.00		NIST Webbook
rinpol	1122.00		NIST Webbook
tb	524.28	K	Joback Method
tc	738.14	K	Joback Method
tf	305.90	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.04	J/mol×K	524.28	Joback Method
cpg	372.80	J/mol×K	559.92	Joback Method
cpg	389.50	J/mol×K	595.57	Joback Method
cpg	405.24	J/mol×K	631.21	Joback Method
cpg	420.13	J/mol×K	666.86	Joback Method
cpg	434.25	J/mol×K	702.50	Joback Method

cpg	447.71	J/mol×K	738.14	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=C4630813&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