Cyclohexanecarboxylic acid, ethyl ester

Other names:	Ethyl cyclohexanecarboxylate
	Ethyl cyclohexylmethanoate
	Ethyl cyclohexanoate
	Ethyl cyclohexanocarboxylate
	Ethyl cyclohexylformate
	NSC 5298
Inchi:	InChI=1S/C9H16O2/c1-2-11-9(10)8-6-4-3-5-7-8/h8H,2-7H2,1H3
InchiKey:	JJOYCHKVKWDMEA-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CCOC(=O)C1CCCCC1
Mol. weight [g/mol]:	156.22
CAS:	3289-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-184.57	kJ/mol	Joback Method
hf	-419.57	kJ/mol	Joback Method
hfus	13.69	kJ/mol	Joback Method
hvap	45.21	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.130		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1105.82		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1108.49		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1174.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1404.00		NIST Webbook

ripol	1413.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1429.00		NIST Webbook
tb	469.70 ± 1.00	K	NIST Webbook
tc	709.61	K	Joback Method
tf	270.73	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.17	J/mol×K	709.61	Joback Method
cpg	385.24	J/mol×K	674.87	Joback Method
cpg	371.51	J/mol×K	640.12	Joback Method
cpg	356.96	J/mol×K	605.38	Joback Method
cpg	341.59	J/mol×K	570.64	Joback Method
cpg	325.39	J/mol×K	535.90	Joback Method
cpg	308.34	J/mol×K	501.16	Joback Method
cpl	271.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0003432	Pa×s	462.75	Joback Method
dvisc	0.0004740	Pa×s	424.35	Joback Method
dvisc	0.0006979	Pa×s	385.94	Joback Method
dvisc	0.0011196	Pa×s	347.54	Joback Method
dvisc	0.0020196	Pa×s	309.13	Joback Method
dvisc	0.0043071	Pa×s	270.73	Joback Method
dvisc	0.0002611	Pa×s	501.16	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=C3289289&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
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume