Ethyl piperidine-4-carboxylate

Other names:	Ethyl isonipecotate
	Piperidine-4-carboxylic acid ethyl ester
	4-Carbethoxypiperidine
	Ethyl 4-piperidinecarboxylate
	4-Piperidinecarboxylic acid, ethyl ester
Inchi:	InChI=1S/C8H15NO2/c1-2-11-8(10)7-3-5-9-6-4-7/h7,9H,2-6H2,1H3
InchiKey:	RUJPPJYDHHAEEK-UHFFFAOYSA-N
Formula:	C8H15NO2
SMILES:	CCOC(=O)C1CCNCC1
Mol. weight [g/mol]:	157.21
CAS:	1126-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-105.28	kJ/mol	Joback Method
hf	-361.12	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	49.75	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.549		Crippen Method
mcvol	130.140	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	477.20	K	NIST Webbook
tc	743.86	K	Joback Method
tf	364.49	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.11	J/mol×K	526.83	Joback Method
cpg	323.36	J/mol×K	563.00	Joback Method
cpg	338.81	J/mol×K	599.17	Joback Method
cpg	353.45	J/mol×K	635.35	Joback Method

cpg	367.28	J/mol×K	671.52	Joback Method
cpg	380.31	J/mol×K	707.69	Joback Method
cpg	392.53	J/mol×K	743.86	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=C1126096&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