

3-Carbethoxy-2-piperidone

Other names:	3-Ethoxycarbonyl-2-piperidone 3-Carbethoxy piperidone-2 3-Piperidinecarboxylic acid, 2-oxo-, ethyl ester Nipecotic acid, 2-oxo-, ethyl ester ethyl 2-oxopiperidine-3-carboxylate
Inchi:	InChI=1S/C8H13NO3/c1-2-12-8(11)6-4-3-5-9-7(6)10/h6H,2-5H2,1H3,(H,9,10)
InchiKey:	DUMNOWYWTAYLJN-UHFFFAOYSA-N
Formula:	C8H13NO3
SMILES:	CCOC(=O)C1CCCNC1=O
Mol. weight [g/mol]:	171.19
CAS:	3731-16-6

Physical Properties

Property code	Value	Unit	Source
gf	-227.87	kJ/mol	Joback Method
hf	-498.82	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hvap	53.99	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.076		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	594.65	K	Joback Method
tc	825.88	K	Joback Method
tf	432.71	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.79	J/molxK	594.65	Joback Method
cpg	351.60	J/molxK	633.19	Joback Method
cpg	366.59	J/molxK	671.73	Joback Method
cpg	380.70	J/molxK	710.26	Joback Method

cpg	393.91	J/mol×K	748.80	Joback Method
cpg	406.17	J/mol×K	787.34	Joback Method
cpg	417.45	J/mol×K	825.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3731166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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