

ETHYL 2-PIPERIDINECARBOXYLATE

Other names:	2-Piperidinecarboxylic acid, ethyl ester ethyl piperidine-2-carboxylate
Inchi:	InChI=1S/C8H15NO2/c1-2-11-8(10)7-5-3-4-6-9-7/h7,9H,2-6H2,1H3
InchiKey:	SZIKRGHFZTYTIT-UHFFFAOYSA-N
Formula:	C8H15NO2
SMILES:	CCOC(=O)C1CCCCN1
Mol. weight [g/mol]:	157.21

Physical Properties

Property code	Value	Unit	Source
hf	-424.73	kJ/mol	Cheméo Relay (1.0)
hfus	20.69	kJ/mol	Joback Method
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-0.47		Cheméo Relay (1.0)
logp	0.692		Crippen Method
mcvol	130.140	ml/mol	McGowan Method
tb	484.97	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C15862723&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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