

Cyclopentanecarboxylic acid, 3-carbamoyl-, methyl ester, cis-

Inchi:	InChI=1S/C8H13NO3/c1-12-8(11)6-3-2-5(4-6)7(9)10/h5-6H,2-4H2,1H3,(H2,9,10)
InchiKey:	NAOJQODZBBRFCP-UHFFFAOYSA-N
Formula:	C8H13NO3
SMILES:	COC(=O)C1CCC(C(N)=O)C1
Mol. weight [g/mol]:	171.19
CAS:	116595-43-8

Physical Properties

Property code	Value	Unit	Source
gf	-251.07	kJ/mol	Joback Method
hf	-491.90	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	59.89	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.061		Crippen Method
mvol	131.710	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	595.74	K	Joback Method
tc	817.59	K	Joback Method
tf	391.93	K	Joback Method
vc	0.482	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.12	J/mol×K	595.74	Joback Method
cpg	358.35	J/mol×K	632.71	Joback Method
cpg	371.71	J/mol×K	669.69	Joback Method
cpg	384.22	J/mol×K	706.66	Joback Method
cpg	395.89	J/mol×K	743.64	Joback Method
cpg	406.74	J/mol×K	780.61	Joback Method
cpg	416.76	J/mol×K	817.59	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=C116595438&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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