

N-Carbomethoxy-N-methylamine

Inchi:

InChI=1S/C3H7NO2/c1-4-3(5)6-2/h1-2H3,(H,4,5)

InchiKey:

NYXHSRNBKJIQQG-UHFFFAOYSA-N

Formula:

C3H7NO2

SMILES:

CNC(=O)OC

Mol. weight [g/mol]:

89.09

Physical Properties

Property code	Value	Unit	Source
af	0.4408		Cheméo Relay (1.0)
hf	-420.12	kJ/mol	Cheméo Relay (1.0)
hfus	11.41	kJ/mol	Joback Method
hvap	48.80	kJ/mol	Cheméo Relay (1.0)
ie	9.75	eV	Cheméo Relay (1.0)
log10ws	0.52		Cheméo Relay (1.0)
logp	-0.028		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
tb	417.86	K	Cheméo Relay (1.0)
tc	594.12	K	Cheméo Relay (1.0)
tf	271.49	K	Cheméo Relay (1.0)
vc	0.257	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.00	J/mol×K	394.50	Joback Method
cpg	135.54	J/mol×K	425.45	Joback Method
cpg	141.91	J/mol×K	456.41	Joback Method
cpg	148.08	J/mol×K	487.36	Joback Method
cpg	154.07	J/mol×K	518.32	Joback Method
cpg	159.85	J/mol×K	549.27	Joback Method
cpg	165.44	J/mol×K	580.23	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C6642304>

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

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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