

CYCLOPENTANECARBOXYLIC ACID, 3-OXO-, METHYL ESTER

Other names:	3-Carbomethoxycyclopentanone
	Methyl 3-oxocyclopentanecarboxylate
Inchi:	InChI=1S/C7H10O3/c1-10-7(9)5-2-3-6(8)4-5/h5H,2-4H2,1H3
InchiKey:	KTGCFXSELRVRFH-UHFFFAOYSA-N
Formula:	C7H10O3
SMILES:	COC(=O)C1CCC(=O)C1
Mol. weight [g/mol]:	142.15

Physical Properties

Property code	Value	Unit	Source
hf	-497.09	kJ/mol	Cheméo Relay (1.0)
hfus	10.12	kJ/mol	Joback Method
hvap	58.09	kJ/mol	Cheméo Relay (1.0)
logp	0.529		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
tb	482.58	K	Cheméo Relay (1.0)
tf	303.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.16	J/mol×K	518.95	Joback Method
cpg	260.76	J/mol×K	556.17	Joback Method
cpg	273.75	J/mol×K	593.38	Joback Method
cpg	286.12	J/mol×K	630.60	Joback Method
cpg	297.83	J/mol×K	667.82	Joback Method
cpg	308.88	J/mol×K	705.03	Joback Method
cpg	319.24	J/mol×K	742.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32811759&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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