

Cyclopentanecarboxylic acid, 1-methyl-, methyl ester

Other names:	Cyclopentanoic acid, 1-methyl, methyl ester
Inchi:	InChI=1S/C8H14O2/c1-8(7(9)10-2)5-3-4-6-8/h3-6H2,1-2H3
InchiKey:	SUCGJXDLZCDFRV-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	COC(=O)C1(C)CCCC1
Mol. weight [g/mol]:	142.20
CAS:	4630-83-5

Physical Properties

Property code	Value	Unit	Source
gf	-186.38	kJ/mol	Joback Method
hf	-377.53	kJ/mol	Joback Method
hfus	6.90	kJ/mol	Joback Method
hvap	41.66	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.740		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	925.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	925.00		NIST Webbook
tb	474.25	K	Joback Method
tc	686.75	K	Joback Method
tf	286.88	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.24	J/molxK	474.25	Joback Method
cpg	279.45	J/molxK	509.67	Joback Method
cpg	293.67	J/molxK	545.08	Joback Method
cpg	307.00	J/molxK	580.50	Joback Method
cpg	319.52	J/molxK	615.92	Joback Method

cpg	331.34	J/mol×K	651.34	Joback Method
cpg	342.56	J/mol×K	686.75	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	432.70	K	96.10	NIST Webbook
tbrp	359.70	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4630835&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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