3-Cyclopentylpropionic acid, methyl ester

Inchi: InChI=1S/C9H16O2/c1-11-9(10)7-6-8-4-2-3-5-8/h8H,2-7H2,1H3
InchiKey: FGPDDJMBTHHHRK-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: COC(=O)CCC1CCCC1
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-172.47	kJ/mol	Joback Method
hf	-413.41	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	45.04	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.130		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
tb	496.89	K	Joback Method
tc	697.79	K	Joback Method
tf	274.25	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.29	J/mol×K	496.89	Joback Method
cpg	324.35	J/mol×K	530.37	Joback Method
cpg	339.64	J/mol×K	563.86	Joback Method
cpg	354.15	J/mol×K	597.34	Joback Method
cpg	367.91	J/mol×K	630.82	Joback Method
cpg	380.94	J/mol×K	664.31	Joback Method
cpg	393.25	J/mol×K	697.79	Joback Method
dvisc	0.0033301	Pa×s	274.25	Joback Method

dvisc	0.0017834	Pa×s	311.36	Joback Method
dvisc	0.0010909	Pa×s	348.46	Joback Method
dvisc	0.0007336	Pa×s	385.57	Joback Method
dvisc	0.0005289	Pa×s	422.68	Joback Method
dvisc	0.0004019	Pa×s	459.78	Joback Method
dvisc	0.0003183	Pa×s	496.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R292512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
dvisc:	Dynamic viscosity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume