

Cyclohexanecarboxylic acid, 4-methoxy-

Inchi:	InChI=1S/C8H14O3/c1-11-7-4-2-6(3-5-7)8(9)10/h6-7H,2-5H2,1H3,(H,9,10)
InchiKey:	WKILSRYNRQGRMA-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	COC1CCC(C(=O)O)CC1
Mol. weight [g/mol]:	158.19

Physical Properties

Property code	Value	Unit	Source
gf	-337.52	kJ/mol	Joback Method
hf	-571.50	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	59.36	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.276		Crippen Method
mcvol	126.030	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
tb	565.79	K	Joback Method
tc	763.42	K	Joback Method
tf	316.04	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.94	J/molxK	565.79	Joback Method
cpg	335.79	J/molxK	598.73	Joback Method
cpg	348.96	J/molxK	631.67	Joback Method
cpg	361.43	J/molxK	664.60	Joback Method
cpg	373.23	J/molxK	697.54	Joback Method
cpg	384.34	J/molxK	730.48	Joback Method
cpg	394.77	J/molxK	763.42	Joback Method
dvisc	0.0085780	Paxs	316.04	Joback Method

dvisc	0.0028126	Paxs	357.67	Joback Method
dvisc	0.0011636	Paxs	399.29	Joback Method
dvisc	0.0005687	Paxs	440.91	Joback Method
dvisc	0.0003145	Paxs	482.54	Joback Method
dvisc	0.0001910	Paxs	524.16	Joback Method
dvisc	0.0001249	Paxs	565.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406189&Units=SI

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

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