Cyclohexanecarboxylic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C14H18O3/c1-16-12-7-9-13(10-8-12)17-14(15)11-5-3-2-4-6-11/h7-11H,2-6H2,
InchiKey: FRLVVPHULLQDHW-UHFFFAOYSA-N
Formula: C14H18O3
SMILES: COc1ccc(OC(=O)C2CCCCC2)cc1
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	-144.69	kJ/mol	Joback Method
hf	-429.93	kJ/mol	Joback Method
hfus	21.48	kJ/mol	Joback Method
hvap	61.69	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.181		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1862.00		NIST Webbook
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tb	669.64	K	Joback Method
tc	902.28	K	Joback Method
tf	388.25	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.12	J/mol×K	669.64	Joback Method
cpg	531.84	J/mol×K	708.41	Joback Method
cpg	549.23	J/mol×K	747.19	Joback Method
cpg	565.30	J/mol×K	785.96	Joback Method
cpg	580.08	J/mol×K	824.73	Joback Method
cpg	593.57	J/mol×K	863.50	Joback Method
cpg	605.80	J/mol×K	902.28	Joback Method
dvisc	0.0013915	Pa×s	388.25	Joback Method

dvisc	0.0007502	Pa×s	435.15	Joback Method
dvisc	0.0004562	Pa×s	482.05	Joback Method
dvisc	0.0003029	Pa×s	528.95	Joback Method
dvisc	0.0002150	Pa×s	575.84	Joback Method
dvisc	0.0001607	Pa×s	622.74	Joback Method
dvisc	0.0001251	Pa×s	669.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307705&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

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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