

Cyclohexanecarboxylic acid, 4-methoxy-, 4-methyl-2-pentyl ester

Inchi:	InChI=1S/C14H26O3/c1-10(2)9-11(3)17-14(15)12-5-7-13(16-4)8-6-12/h10-13H,5-9H2,1-
InchiKey:	WZFNGOZLQHGJCK-UHFFFAOYSA-N
Formula:	C14H26O3
SMILES:	COC1CCC(C(=O)OC(C)CC(C)C)CC1
Mol. weight [g/mol]:	242.35

Physical Properties

Property code	Value	Unit	Source
gf	-260.06	kJ/mol	Joback Method
hf	-685.89	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.169		Crippen Method
mvol	210.570	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	1642.00		NIST Webbook
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tb	632.43	K	Joback Method
tc	832.18	K	Joback Method
tf	315.07	K	Joback Method
vc	0.781	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.07	J/mol×K	632.43	Joback Method
cpg	684.63	J/mol×K	798.88	Joback Method
cpg	668.30	J/mol×K	765.59	Joback Method
cpg	650.88	J/mol×K	732.30	Joback Method
cpg	632.37	J/mol×K	699.01	Joback Method
cpg	612.77	J/mol×K	665.72	Joback Method
cpg	699.88	J/mol×K	832.18	Joback Method
dvisc	0.0001298	Paxs	632.43	Joback Method

dvisc	0.0001750	Paxs	579.54	Joback Method
dvisc	0.0002506	Paxs	526.64	Joback Method
dvisc	0.0003888	Paxs	473.75	Joback Method
dvisc	0.0006735	Paxs	420.86	Joback Method
dvisc	0.0013664	Paxs	367.96	Joback Method
dvisc	0.0035155	Paxs	315.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406193&Units=SI
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

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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