Cyclohexanecarboxylic acid, 4-methoxy-, pentyl ester

Inchi: InChI=1S/C13H24O3/c1-3-4-5-10-16-13(14)11-6-8-12(15-2)9-7-11/h11-12H,3-10H2,1-2H

InchiKey: SOQUDWGSKKWGSW-UHFFFAOYSA-N

Formula: C13H24O3

SMILES: CCCCCOC(=O)C1CCC(OC)CC1

Mol. weight [g/mol]: 228.33

Physical Properties

Property code	Value	Unit	Source
gf	-263.60	kJ/mol	Joback Method
hf	-654.69	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	56.22	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.925		Crippen Method
mcvol	196.480	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
tb	610.43	K	Joback Method
tc	805.42	K	Joback Method
tf	333.80	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.02	J/mol×K	610.43	Joback Method
cpg	556.53	J/mol×K	642.93	Joback Method
cpg	575.08	J/mol×K	675.43	Joback Method
cpg	592.67	J/mol×K	707.92	Joback Method
cpg	609.30	J/mol×K	740.42	Joback Method
cpg	624.97	J/mol×K	772.92	Joback Method
cpg	639.68	J/mol×K	805.42	Joback Method
dvisc	0.0021968	Pa×s	333.80	Joback Method

dvisc	0.0011004	Pa×s	379.90	Joback Method
dvisc	0.0006402	Pa×s	426.01	Joback Method
dvisc	0.0004140	Pa×s	472.12	Joback Method
dvisc	0.0002893	Pa×s	518.22	Joback Method
dvisc	0.0002144	Pa×s	564.32	Joback Method
dvisc	0.0001662	Pa×s	610.43	Joback Method

Sources

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=U406192&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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