Cyclohexanecarboxylic acid, 4-methoxy-, heptyl ester

Inchi: InChI=1S/C15H28O3/c1-3-4-5-6-7-12-18-15(16)13-8-10-14(17-2)11-9-13/h13-14H,3-12H

InchiKey: MHTOVMNNTKKLEZ-UHFFFAOYSA-N

Formula: C15H28O3

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

Mol. weight [g/mol]: 256.38

Physical Properties

Property code	Value	Unit	Source
gf	-246.76	kJ/mol	Joback Method
hf	-695.97	kJ/mol	Joback Method
hfus	31.49	kJ/mol	Joback Method
hvap	60.67	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.705		Crippen Method
mcvol	224.660	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
tb	656.19	K	Joback Method
tc	846.89	K	Joback Method
tf	356.34	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.96	J/mol×K	656.19	Joback Method
cpg	667.14	J/mol×K	687.97	Joback Method
cpg	686.28	J/mol×K	719.76	Joback Method
cpg	704.39	J/mol×K	751.54	Joback Method
cpg	721.47	J/mol×K	783.32	Joback Method
cpg	737.53	J/mol×K	815.11	Joback Method
cpg	752.57	J/mol×K	846.89	Joback Method
dvisc	0.0019602	Pa×s	356.34	Joback Method

dvisc	0.0009529	Pa×s	406.31	Joback Method
dvisc	0.0005425	Pa×s	456.29	Joback Method
dvisc	0.0003452	Pa×s	506.26	Joback Method
dvisc	0.0002382	Pa×s	556.24	Joback Method
dvisc	0.0001748	Pa×s	606.21	Joback Method
dvisc	0.0001344	Pa×s	656.19	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=U406195&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