Cyclohexanecarboxylic acid, 4-methoxy-, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H22O3/c1-4-6-12(5-2)17-14(15)11-7-9-13(16-3)10-8-11/h11-13H,5,7-10H2

InchiKey: OEUKEWKCXLFYRX-UHFFFAOYSA-N

Formula: C14H22O3

SMILES: CC#CC(CC)OC(=O)C1CCC(OC)CC1

Mol. weight [g/mol]: 238.32

Physical Properties

Property code	Value	Unit	Source
gf	-54.82	kJ/mol	Joback Method
hf	-408.31	kJ/mol	Joback Method
hfus	28.50	kJ/mol	Joback Method
hvap	60.21	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.537		Crippen Method
mcvol	201.970	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1709.00		NIST Webbook
tb	641.87	K	Joback Method
tc	859.68	K	Joback Method
tf	436.17	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.19	J/mol×K	641.87	Joback Method
cpg	571.31	J/mol×K	678.17	Joback Method
cpg	590.27	J/mol×K	714.47	Joback Method
cpg	608.06	J/mol×K	750.78	Joback Method
cpg	624.69	J/mol×K	787.08	Joback Method
cpg	640.16	J/mol×K	823.38	Joback Method
cpg	654.46	J/mol×K	859.68	Joback Method

Sources

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=U406990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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