Cyclohexanecarboxylic acid, 4-methoxy-, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C17H28O3/c1-5-6-7-16(12-13(2)3)20-17(18)14-8-10-15(19-4)11-9-14/h13-16H

InchiKey: KXPXHFIPJYWTCS-UHFFFAOYSA-N

Formula: C17H28O3

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

Mol. weight [g/mol]: 280.40

Physical Properties

Property code	Value	Unit	Source
gf	-32.00	kJ/mol	Joback Method
hf	-475.51	kJ/mol	Joback Method
hfus	32.74	kJ/mol	Joback Method
hvap	66.50	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.563		Crippen Method
mcvol	244.240	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tb	710.07	K	Joback Method
tc	921.73	K	Joback Method
tf	454.98	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.90	J/mol×K	710.07	Joback Method
cpg	740.03	J/mol×K	745.35	Joback Method
cpg	759.86	J/mol×K	780.62	Joback Method
cpg	778.37	J/mol×K	815.90	Joback Method
cpg	795.58	J/mol×K	851.18	Joback Method
cpg	811.50	J/mol×K	886.45	Joback Method
cpg	826.14	J/mol×K	921.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406992&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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