Cyclohexanecarboxylic acid, 4-methoxy-, tridec-2-yn-1-yl ester

Inchi: InChI=1S/C21H36O3/c1-3-4-5-6-7-8-9-10-11-12-13-18-24-21(22)19-14-16-20(23-2)17-15

InchiKey: GFTCBSMWSXTZQA-UHFFFAOYSA-N

Formula: C21H36O3

SMILES: CCCCCCCCCCC#CCOC(=O)C1CCC(OC)CC1

Mol. weight [g/mol]: 336.51

Physical Properties

Property code	Value	Unit	Source
gf	6.56	kJ/mol	Joback Method
hf	-547.51	kJ/mol	Joback Method
hfus	50.15	kJ/mol	Joback Method
hvap	76.18	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.269		Crippen Method
mcvol	300.600	ml/mol	McGowan Method
pc	1211.51	kPa	Joback Method
rinpol	2492.00		NIST Webbook
rinpol	2492.00		NIST Webbook
tb	802.47	K	Joback Method
tc	1001.70	K	Joback Method
tf	530.06	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.75	J/mol×K	802.47	Joback Method
cpg	976.44	J/mol×K	835.68	Joback Method
cpg	995.78	J/mol×K	868.88	Joback Method
cpg	1013.80	J/mol×K	902.09	Joback Method
cpg	1030.51	J/mol×K	935.29	Joback Method
cpg	1045.92	J/mol×K	968.50	Joback Method
cpg	1060.06	J/mol×K	1001.70	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=U406995&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
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