Cyclohexanecarboxylic acid, 4-methoxy-, undec-2-en-1-yl ester

Inchi: InChI=1S/C19H34O3/c1-3-4-5-6-7-8-9-10-11-16-22-19(20)17-12-14-18(21-2)15-13-17/h1

InchiKey: JTKJPTIFEYXAAC-ZHACJKMWSA-N

Formula: C19H34O3

SMILES: CCCCCCCCC=CCOC(=O)C1CCC(OC)CC1

Mol. weight [g/mol]: 310.47

Physical Properties

Property code	Value	Unit	Source
gf	-132.86	kJ/mol	Joback Method
hf	-661.31	kJ/mol	Joback Method
hfus	42.05	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.042		Crippen Method
mcvol	276.720	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2258.00		NIST Webbook
rinpol	2258.00		NIST Webbook
tb	751.87	K	Joback Method
tc	943.56	K	Joback Method
tf	396.34	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.50	J/mol×K	751.87	Joback Method
cpg	948.40	J/mol×K	911.61	Joback Method
cpg	932.51	J/mol×K	879.67	Joback Method
cpg	915.49	J/mol×K	847.72	Joback Method
cpg	897.34	J/mol×K	815.77	Joback Method
cpg	878.02	J/mol×K	783.82	Joback Method
cpg	963.19	J/mol×K	943.56	Joback Method
dvisc	0.0000718	Pa×s	751.87	Joback Method

dvisc	0.0000949	Pa×s	692.61	Joback Method
dvisc	0.0001319	Pa×s	633.36	Joback Method
dvisc	0.0001964	Pa×s	574.11	Joback Method
dvisc	0.0003206	Pa×s	514.85	Joback Method
dvisc	0.0005941	Pa×s	455.60	Joback Method
dvisc	0.0013244	Pa×s	396.34	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=U406994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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