Cyclohexanecarboxylic acid, 4-methoxy-, 2,7-dimethyloct-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C18H28O3/c1-13(2)6-9-17(12-14(3)4)21-18(19)15-7-10-16(20-5)11-8-15/h14-1

InchiKey: DHFKPFBAKHXUIT-UHFFFAOYSA-N

Formula: C18H28O3

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

Mol. weight [g/mol]: 292.41

Physical Properties

Property code	Value	Unit	Source
gf	55.71	kJ/mol	Joback Method
hf	-380.51	kJ/mol	Joback Method
hfus	32.74	kJ/mol	Joback Method
hvap	68.13	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.729		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	729.51	K	Joback Method
tc	944.82	K	Joback Method
tf	450.53	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.47	J/mol×K	729.51	Joback Method
cpg	772.51	J/mol×K	765.39	Joback Method
cpg	792.17	J/mol×K	801.28	Joback Method
cpg	810.47	J/mol×K	837.16	Joback Method
cpg	827.43	J/mol×K	873.05	Joback Method
cpg	843.06	J/mol×K	908.93	Joback Method
cpg	857.38	J/mol×K	944.82	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=U406993&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