Cyclopropanecarboxylic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C15H22O2/c1-5-6-12(4)14(10-7-11(2)3)17-15(16)13-8-9-13/h12-14H,2,5-6,8-9

InchiKey: VFJRVZGRSIWNJD-UHFFFAOYSA-N

Formula: C15H22O2

SMILES: C=C(C)C#CC(OC(=O)C1CC1)C(C)CCC

Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	179.46	kJ/mol	Joback Method
hf	-147.55	kJ/mol	Joback Method
hfus	29.01	kJ/mol	Joback Method
hvap	58.84	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.324		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1528.00		NIST Webbook
tb	630.31	K	Joback Method
tc	838.76	K	Joback Method
tf	409.29	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.42	J/mol×K	630.31	Joback Method
cpg	563.38	J/mol×K	665.05	Joback Method
cpg	580.33	J/mol×K	699.79	Joback Method
cpg	596.30	J/mol×K	734.54	Joback Method
cpg	611.35	J/mol×K	769.28	Joback Method
cpg	625.54	J/mol×K	804.02	Joback Method
cpg	638.90	J/mol×K	838.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299380&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