Cyclopropanecarboxylic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C13H20O2/c1-4-5-6-12(9-10(2)3)15-13(14)11-7-8-11/h10-12H,4,7-9H2,1-3H3

InchiKey: LELZXSOBOUZPNC-UHFFFAOYSA-N

Formula: C13H20O2

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

Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	83.33	kJ/mol	Joback Method
hf	-221.91	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	54.98	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.768		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	587.99	K	Joback Method
tc	795.45	K	Joback Method
tf	402.47	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.26	J/mol×K	587.99	Joback Method
cpg	481.55	J/mol×K	622.57	Joback Method
cpg	497.90	J/mol×K	657.14	Joback Method
cpg	513.34	J/mol×K	691.72	Joback Method
cpg	527.91	J/mol×K	726.30	Joback Method
cpg	541.66	J/mol×K	760.88	Joback Method
cpg	554.61	J/mol×K	795.45	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=U299378&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

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