Cyclopropanecarboxylic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C10H14O2/c1-3-5-9(4-2)12-10(11)8-6-7-8/h8-9H,4,6-7H2,1-2H3
InchiKey: VIHFMWLNZWQDGK-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC#CC(CC)OC(=O)C1CC1
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	60.51	kJ/mol	Joback Method
hf	-154.71	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	48.69	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.742		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1194.00		NIST Webbook
tb	519.79	K	Joback Method
tc	732.90	K	Joback Method
tf	383.66	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.45	J/mol×K	519.79	Joback Method
cpg	335.16	J/mol×K	555.31	Joback Method
cpg	349.07	J/mol×K	590.83	Joback Method
cpg	362.21	J/mol×K	626.35	Joback Method
cpg	374.61	J/mol×K	661.86	Joback Method
cpg	386.30	J/mol×K	697.38	Joback Method
cpg	397.32	J/mol×K	732.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299376&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

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

Latest version available from:
https://www.chemeo.com/cid/52-383-9/Cyclopropanecarboxylic-acid-hex-4-yn-3-yl-ester.pdf
Generated by Cheméo on 2024-04-18 15:13:34.844818665 +0000 UTC m=+15742463.765395981.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.