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

Inchi: InChI=1S/C11H16O2/c1-3-6-10(4-2)13-11(12)9-7-5-8-9/h9-10H,4-5,7-8H2,1-2H3
InchiKey: YQYKIUIBLHLILR-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CC#CC(CC)OC(=O)C1CCC1
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	56.83	kJ/mol	Joback Method
hf	-181.51	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	51.09	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.132		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1297.00		NIST Webbook
tb	546.94	K	Joback Method
tc	764.22	K	Joback Method
tf	391.41	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.11	J/mol×K	546.94	Joback Method
cpg	383.61	J/mol×K	583.15	Joback Method
cpg	399.21	J/mol×K	619.37	Joback Method
cpg	413.91	J/mol×K	655.58	Joback Method
cpg	427.77	J/mol×K	691.79	Joback Method
cpg	440.79	J/mol×K	728.01	Joback Method
cpg	453.03	J/mol×K	764.22	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=U299131&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

Latest version available from:
https://www.chemeo.com/cid/45-350-3/Cyclobutanecarboxylic-acid-hex-4-yn-3-yl-ester.pdf
Generated by Cheméo on 2024-04-17 02:36:14.810119248 +0000 UTC m=+15610623.730696563.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.