

Cyclopropanecarboxylic acid, pent-2-en-4-ynyl ester

Inchi:	InChI=1S/C9H10O2/c1-2-3-4-7-11-9(10)8-5-6-8/h1,3-4,8H,5-7H2
InchiKey:	RUKMQPUIALQPLK-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	C#CC=CCOC(=O)C1CC1
Mol. weight [g/mol]:	150.17

Physical Properties

Property code	Value	Unit	Source
gf	155.02	kJ/mol	Joback Method
hf	8.03	kJ/mol	Joback Method
hfus	23.16	kJ/mol	Joback Method
hvap	44.51	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.129		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	976.00		NIST Webbook
tb	482.63	K	Joback Method
tc	692.42	K	Joback Method
tf	323.18	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.56	J/mol×K	482.63	Joback Method
cpg	271.02	J/mol×K	517.59	Joback Method
cpg	282.68	J/mol×K	552.56	Joback Method
cpg	293.58	J/mol×K	587.52	Joback Method
cpg	303.77	J/mol×K	622.49	Joback Method
cpg	313.31	J/mol×K	657.45	Joback Method
cpg	322.25	J/mol×K	692.42	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=U299375&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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