Cyclobutanecarboxylic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C10H14O2/c1-3-5-8(2)12-10(11)9-6-4-7-9/h8-9H,4,6-7H2,1-2H3
InchiKey: MRQLUWIUYAYLSZ-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC#CC(C)OC(=O)C1CCC1
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	48.41	kJ/mol	Joback Method
hf	-160.87	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	48.86	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.742		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
tb	524.06	K	Joback Method
tc	745.14	K	Joback Method
tf	380.14	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.55	J/mol×K	524.06	Joback Method
cpg	336.22	J/mol×K	560.91	Joback Method
cpg	351.03	J/mol×K	597.75	Joback Method
cpg	364.99	J/mol×K	634.60	Joback Method
cpg	378.13	J/mol×K	671.45	Joback Method
cpg	390.49	J/mol×K	708.29	Joback Method
cpg	402.08	J/mol×K	745.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299128&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume