endo-2-(1,1-Dimethylprop-2-ynyloxycarbonyl)bicy

Inchi: InChI=1S/C13H16O2/c1-4-13(2,3)15-12(14)11-8-9-5-6-10(11)7-9/h1,5-6,9-11H,7-8H2,2-
InchiKey: CKKZVCNCQWQXIL-FBKFWFMHSA-N
Formula: C13H16O2
SMILES: C#CC(C)(C)OC(=O)C1CC2C=CC1C2
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	182.22	kJ/mol	Joback Method
hf	-96.42	kJ/mol	Joback Method
hfus	24.24	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.154		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1268.00		NIST Webbook
rinpol	1268.00		NIST Webbook
tb	572.26	K	Joback Method
tc	797.55	K	Joback Method
tf	386.70	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.35	J/mol×K	572.26	Joback Method
cpg	450.41	J/mol×K	609.81	Joback Method
cpg	467.15	J/mol×K	647.36	Joback Method
cpg	482.65	J/mol×K	684.91	Joback Method
cpg	497.03	J/mol×K	722.46	Joback Method
cpg	510.37	J/mol×K	760.01	Joback Method
cpg	522.79	J/mol×K	797.55	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R507443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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