endo-2-(Prop-2-ynyloxycarbonyl)bicyclo[2.2.1]hep

Inchi: InChI=1S/C11H12O2/c1-2-5-13-11(12)10-7-8-3-4-9(10)6-8/h1,3-4,8-10H,5-7H2/t8-,9?,10
InchiKey: WITAKKIPQQHPBU-FIBVVXLUSA-N
Formula: C11H12O2
SMILES: C#CCOC(=O)C1CC2C=CC1C2
Mol. weight [g/mol]: 176.21

Physical Properties

Property code	Value	Unit	Source
gf	162.54	kJ/mol	Joback Method
hf	-46.39	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	49.08	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.375		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
tb	529.73	K	Joback Method
tc	749.07	K	Joback Method
tf	361.74	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.65	J/mol×K	529.73	Joback Method
cpg	349.39	J/mol×K	566.29	Joback Method
cpg	364.06	J/mol×K	602.84	Joback Method
cpg	377.75	J/mol×K	639.40	Joback Method
cpg	390.51	J/mol×K	675.96	Joback Method
cpg	402.41	J/mol×K	712.52	Joback Method
cpg	413.52	J/mol×K	749.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R507458&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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