Cyclohexanol, 1-ethynyl-, acetate

Other names: 1-ethynylcyclohexyl acetate
Inchi: InChI=1S/C10H14O2/c1-3-10(12-9(2)11)7-5-4-6-8-10/h1H,4-8H2,2H3
InchiKey: YASSLXHVJQGNOK-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: C#CC1(OC(C)=O)CCCCC1
Mol. weight [g/mol]: 166.22
CAS: 5240-32-4

Physical Properties

Property code	Value	Unit	Source
gf	41.43	kJ/mol	Joback Method
hf	-133.07	kJ/mol	Joback Method
hfus	12.96	kJ/mol	Joback Method
hvap	46.15	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	1.886		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	1136.70		NIST Webbook
tb	514.40	K	Joback Method
tc	744.43	K	Joback Method
tf	352.87	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.97	J/mol×K	514.40	Joback Method
cpg	335.52	J/mol×K	552.74	Joback Method
cpg	350.93	J/mol×K	591.08	Joback Method
cpg	365.33	J/mol×K	629.42	Joback Method
cpg	378.85	J/mol×K	667.76	Joback Method
cpg	391.60	J/mol×K	706.10	Joback Method
cpg	403.72	J/mol×K	744.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5240324&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume