(Z)-Deca-8-en-4,6-diyn-1-yl acetate

Inchi: InChI=1S/C12H14O2/c1-3-4-5-6-7-8-9-10-11-14-12(2)13/h3-4H,9-11H2,1-2H3/b4-3-
InchiKey: POFUIXIUNQEQNM-ARJAWSKDSA-N
Formula: C12H14O2
SMILES: CC=CC#CC#CCCCOC(C)=O
Mol. weight [g/mol]: 190.24
CAS: 6131-31-3

Physical Properties

Property code	Value	Unit	Source
gf	302.06	kJ/mol	Joback Method
hf	126.01	kJ/mol	Joback Method
hfus	36.07	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	1.913		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1598.20		NIST Webbook
tb	572.41	K	Joback Method
tc	793.55	K	Joback Method
tf	504.28	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.31	J/mol×K	572.41	Joback Method
cpg	385.25	J/mol×K	609.27	Joback Method
cpg	398.48	J/mol×K	646.12	Joback Method
cpg	411.01	J/mol×K	682.98	Joback Method
cpg	422.86	J/mol×K	719.84	Joback Method
cpg	434.05	J/mol×K	756.70	Joback Method
cpg	444.61	J/mol×K	793.55	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=C6131313&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