Oct-3-enoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H22O2/c1-4-7-8-9-10-12-14(15)16-13(6-3)11-5-2/h9-10,13H,4,6-8,12H2,1-
InchiKey: UKWYAJGZGAHXMW-MDZDMXLPSA-N
Formula: C14H22O2
SMILES: CC#CC(CC)OC(=O)CC=CCCCC
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	113.66	kJ/mol	Joback Method
hf	-192.85	kJ/mol	Joback Method
hfus	34.60	kJ/mol	Joback Method
hvap	57.64	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.468		Crippen Method
mcvol	202.660	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
tb	608.73	K	Joback Method
tc	804.21	K	Joback Method
tf	405.72	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.80	J/mol×K	608.73	Joback Method
cpg	525.18	J/mol×K	641.31	Joback Method
cpg	540.76	J/mol×K	673.89	Joback Method
cpg	555.56	J/mol×K	706.47	Joback Method
cpg	569.61	J/mol×K	739.05	Joback Method
cpg	582.93	J/mol×K	771.63	Joback Method
cpg	595.55	J/mol×K	804.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406949&Units=SI

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