Dec-4,6,8-triyn-2-enoic acid, methyl ester

Inchi: InChI=1S/C11H8O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h9-10H,1-2H3/b10-9+
InchiKey: LBAVIXQTLKRIGP-MDZDMXLPSA-N
Formula: C11H8O2
SMILES: CC#CC#CC#CC=CC(=O)OC
Mol. weight [g/mol]: 172.18

Physical Properties

Property code	Value	Unit	Source
gf	496.44	kJ/mol	Joback Method
hf	418.95	kJ/mol	Joback Method
hfus	36.60	kJ/mol	Joback Method
hvap	55.65	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	0.746		Crippen Method
mcvol	143.190	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	558.53	K	Joback Method
tc	814.21	K	Joback Method
tf	599.11	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.58	J/mol×K	558.53	Joback Method
cpg	299.35	J/mol×K	601.14	Joback Method
cpg	310.47	J/mol×K	643.76	Joback Method
cpg	320.96	J/mol×K	686.37	Joback Method
cpg	330.83	J/mol×K	728.98	Joback Method
cpg	340.10	J/mol×K	771.60	Joback Method
cpg	348.79	J/mol×K	814.21	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=R419282&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