

Methyl (Z)-dec-2-en-4,6-diynoate

Other names:	Lachnophyllum ester, cis (Z)-Lachnophyllum acid, methyl ester 2-Decene-4,6-diynoic acid, methyl ester, (Z)- cis-Lachnophyllum ester (Z)-2-Lachnophyllum ester
Inchi:	InChI=1S/C11H12O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h9-10H,3-4H2,1-2H3/b10-9-
InchiKey:	LWONXTYZMYZRSU-KTKRTIGZSA-N
Formula:	C11H12O2
SMILES:	CCCC#CC#CC=CC(=O)OC
Mol. weight [g/mol]:	176.21
CAS:	505-01-1

Physical Properties

Property code	Value	Unit	Source
gf	293.64	kJ/mol	Joback Method
hf	146.65	kJ/mol	Joback Method
hfus	33.48	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	1.522		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1502.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1504.00		NIST Webbook
ripol	2250.00		NIST Webbook
tb	549.53	K	Joback Method
tc	774.76	K	Joback Method
tf	493.01	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.44	J/molxK	549.53	Joback Method
cpg	338.42	J/molxK	587.07	Joback Method
cpg	350.74	J/molxK	624.61	Joback Method
cpg	362.41	J/molxK	662.15	Joback Method
cpg	373.45	J/molxK	699.69	Joback Method
cpg	383.89	J/molxK	737.22	Joback Method
cpg	393.73	J/molxK	774.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C505011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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