5-Decynedioic acid, dimethyl ester

Other names: Dec-5-ynedioic acid dimethyl ester
Inchi: InChI=1S/C12H18O4/c1-15-11(13)9-7-5-3-4-6-8-10-12(14)16-2/h5-10H2,1-2H3
InchiKey: PUPSLSCNSGWMAI-UHFFFAOYSA-N
Formula: C12H18O4
SMILES: COC(=O)CCCC#CCCCC(=O)OC
Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
gf	-214.88	kJ/mol	Joback Method
hf	-508.31	kJ/mol	Joback Method
hfus	35.53	kJ/mol	Joback Method
hvap	62.77	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.676		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	635.54	K	Joback Method
tc	830.62	K	Joback Method
tf	475.42	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.63	J/mol×K	635.54	Joback Method
cpg	488.55	J/mol×K	668.05	Joback Method
cpg	501.81	J/mol×K	700.57	Joback Method
cpg	514.41	J/mol×K	733.08	Joback Method
cpg	526.34	J/mol×K	765.59	Joback Method
cpg	537.60	J/mol×K	798.11	Joback Method

cpg	548.19	J/mol×K	830.62	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=R106406&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