

cis-5-Dodecenoic acid, methyl ester

Inchi:	InChI=1S/C13H24O2/c1-3-4-5-6-7-8-9-10-11-12-13(14)15-2/h8-9H,3-7,10-12H2,1-2H3/b
InchiKey:	COACURUOBAVMFJ-HJWRWDBZSA-N
Formula:	C13H24O2
SMILES:	CCCCCCC=CCCCC(=O)OC
Mol. weight [g/mol]:	212.33

Physical Properties

Property code	Value	Unit	Source
gf	-95.12	kJ/mol	Joback Method
hf	-439.23	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	53.65	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.856		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1503.30		NIST Webbook
rinpol	1503.30		NIST Webbook
rinpol	1504.30		NIST Webbook
tb	577.29	K	Joback Method
tc	752.37	K	Joback Method
tf	303.35	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.80	J/molxK	577.29	Joback Method
cpg	568.82	J/molxK	723.19	Joback Method
cpg	555.52	J/molxK	694.01	Joback Method
cpg	541.59	J/molxK	664.83	Joback Method
cpg	527.01	J/molxK	635.65	Joback Method
cpg	511.75	J/molxK	606.47	Joback Method
cpg	581.49	J/molxK	752.37	Joback Method

dvisc	0.0001450	Paxs	577.29	Joback Method
dvisc	0.0001917	Paxs	531.63	Joback Method
dvisc	0.0002673	Paxs	485.98	Joback Method
dvisc	0.0003991	Paxs	440.32	Joback Method
dvisc	0.0006538	Paxs	394.66	Joback Method
dvisc	0.0012188	Paxs	349.01	Joback Method
dvisc	0.0027407	Paxs	303.35	Joback Method

Sources

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=U333123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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