

Ethyl 2,6 (Z,E)-dodecadienoate

Inchi:	InChI=1S/C14H24O2/c1-3-5-6-7-8-9-10-11-12-13-14(15)16-4-2/h8-9,12-13H,3-7,10-11H
InchiKey:	AASSLPGKTZCKLS-FRGMPSNRSA-N
Formula:	C14H24O2
SMILES:	CCCCC=CCCC=CC(=O)OCC
Mol. weight [g/mol]:	224.34

Physical Properties

Property code	Value	Unit	Source
gf	-6.48	kJ/mol	Joback Method
hf	-342.65	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	55.83	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.022		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
ripol	2000.00		NIST Webbook
tb	604.33	K	Joback Method
tc	784.52	K	Joback Method
tf	309.54	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.63	J/molxK	604.33	Joback Method
cpg	600.86	J/molxK	754.48	Joback Method
cpg	587.61	J/molxK	724.45	Joback Method
cpg	573.70	J/molxK	694.42	Joback Method
cpg	559.08	J/molxK	664.39	Joback Method
cpg	543.73	J/molxK	634.36	Joback Method
cpg	613.47	J/molxK	784.52	Joback Method

dvisc	0.0001119	Paxs	604.33	Joback Method
dvisc	0.0001489	Paxs	555.20	Joback Method
dvisc	0.0002093	Paxs	506.07	Joback Method
dvisc	0.0003167	Paxs	456.94	Joback Method
dvisc	0.0005296	Paxs	407.80	Joback Method
dvisc	0.0010193	Paxs	358.67	Joback Method
dvisc	0.0024152	Paxs	309.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341743&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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