

Trans-2, cis-4-dodecadienoic acid, methyl ester

Inchi:	InChI=1S/C13H22O2/c1-3-4-5-6-7-8-9-10-11-12-13(14)15-2/h9-12H,3-8H2,1-2H3/b10-9-
InchiKey:	FWDIWEBRLBVZRE-XAZJVICWSA-N
Formula:	C13H22O2
SMILES:	CCCCCCCC=CC=CC(=O)OC
Mol. weight [g/mol]:	210.31
CAS:	39924-47-5

Physical Properties

Property code	Value	Unit	Source
gf	-14.90	kJ/mol	Joback Method
hf	-322.01	kJ/mol	Joback Method
hfus	32.62	kJ/mol	Joback Method
hvap	53.60	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.632		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
tb	581.45	K	Joback Method
tc	763.24	K	Joback Method
tf	298.27	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.55	J/molxK	581.45	Joback Method
cpg	492.11	J/molxK	611.75	Joback Method
cpg	506.92	J/molxK	642.05	Joback Method
cpg	521.03	J/molxK	672.35	Joback Method
cpg	534.46	J/molxK	702.64	Joback Method
cpg	547.24	J/molxK	732.94	Joback Method
cpg	559.41	J/molxK	763.24	Joback Method
dvisc	0.0025562	Paxs	298.27	Joback Method
dvisc	0.0010928	Paxs	345.47	Joback Method

dvisc	0.0005731	Paxs	392.66	Joback Method
dvisc	0.0003452	Paxs	439.86	Joback Method
dvisc	0.0002294	Paxs	487.06	Joback Method
dvisc	0.0001638	Paxs	534.25	Joback Method
dvisc	0.0001236	Paxs	581.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39924475&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
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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