Dodecanoic acid, 2-hexen-1-yl ester

Inchi: InChI=1S/C18H34O2/c1-3-5-7-9-10-11-12-13-14-16-18(19)20-17-15-8-6-4-2/h8,15H,3-7,
InchiKey: RTTISBGEPJMJAZ-OVCLIPMQSA-N
Formula: C18H34O2
SMILES: CCCC=CCOC(=O)CCCCCCCCCCC
Mol. weight [g/mol]: 282.46

Physical Properties

Property code	Value	Unit	Source
gf	-53.02	kJ/mol	Joback Method
hf	-542.43	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	64.78	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.807		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
tb	691.69	K	Joback Method
tc	864.16	K	Joback Method
tf	359.70	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.00	J/mol×K	691.69	Joback Method
cpg	786.32	J/mol×K	720.43	Joback Method
cpg	803.81	J/mol×K	749.18	Joback Method
cpg	820.48	J/mol×K	777.92	Joback Method
cpg	836.37	J/mol×K	806.67	Joback Method
cpg	851.50	J/mol×K	835.41	Joback Method
cpg	865.91	J/mol×K	864.16	Joback Method
dvisc	0.0018910	Pa×s	359.70	Joback Method
dvisc	0.0007915	Pa×s	415.03	Joback Method
dvisc	0.0004066	Pa×s	470.36	Joback Method

dvisc	0.0002403	Pa×s	525.70	Joback Method
dvisc	0.0001570	Pa×s	581.03	Joback Method
dvisc	0.0001105	Pa×s	636.36	Joback Method
dvisc	0.0000822	Pa×s	691.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U159970&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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