Isobutyl (E)-7,9-decadienoate

Inchi: InChI=1S/C14H24O2/c1-4-5-6-7-8-9-10-11-14(15)16-12-13(2)3/h4-6,13H,1,7-12H2,2-3H
InchiKey: SDIYVRQARRNBCN-AATRIKPKSA-N
Formula: C14H24O2
SMILES: C=CC=CCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	-1.30	kJ/mol	Joback Method
hf	-339.72	kJ/mol	Joback Method
hfus	30.20	kJ/mol	Joback Method
hvap	54.81	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.878		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	1572.00		NIST Webbook
rinpol	1572.00		NIST Webbook
tb	596.41	K	Joback Method
tc	776.03	K	Joback Method
tf	297.86	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.48	J/mol×K	596.41	Joback Method
cpg	542.80	J/mol×K	626.35	Joback Method
cpg	558.37	J/mol×K	656.28	Joback Method
cpg	573.20	J/mol×K	686.22	Joback Method
cpg	587.32	J/mol×K	716.16	Joback Method
cpg	600.75	J/mol×K	746.09	Joback Method
cpg	613.52	J/mol×K	776.03	Joback Method
dvisc	0.0033392	Pa×s	297.86	Joback Method

dvisc	0.0013108	Pa×s	347.62	Joback Method
dvisc	0.0006503	Pa×s	397.38	Joback Method
dvisc	0.0003771	Pa×s	447.14	Joback Method
dvisc	0.0002439	Pa×s	496.89	Joback Method
dvisc	0.0001708	Pa×s	546.65	Joback Method
dvisc	0.0001269	Pa×s	596.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R556613&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume