isobutyl 7-octenoate

Inchi: InChI=1S/C12H22O2/c1-4-5-6-7-8-9-12(13)14-10-11(2)3/h4,11H,1,5-10H2,2-3H3
InchiKey: VXCSHKJRSMDDCU-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: C=CCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-98.36	kJ/mol	Joback Method
hf	-415.66	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	50.40	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.322		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
ripol	1591.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1591.00		NIST Webbook
tb	546.49	K	Joback Method
tc	722.36	K	Joback Method
tf	280.40	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.62	J/mol×K	546.49	Joback Method
cpg	460.13	J/mol×K	575.80	Joback Method
cpg	474.98	J/mol×K	605.11	Joback Method
cpg	489.19	J/mol×K	634.42	Joback Method
cpg	502.77	J/mol×K	663.74	Joback Method

cpg	515.75	J/mol×K	693.05	Joback Method
cpg	528.12	J/mol×K	722.36	Joback Method
dvisc	0.0039999	Pa×s	280.40	Joback Method
dvisc	0.0016799	Pa×s	324.75	Joback Method
dvisc	0.0008691	Pa×s	369.10	Joback Method
dvisc	0.0005179	Pa×s	413.44	Joback Method
dvisc	0.0003412	Pa×s	457.79	Joback Method
dvisc	0.0002419	Pa×s	502.14	Joback Method
dvisc	0.0001814	Pa×s	546.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313703&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume