isobutyl 5-octenoate

Inchi: InChI=1S/C12H22O2/c1-4-5-6-7-8-9-12(13)14-10-11(2)3/h5-6,11H,4,7-10H2,1-3H3/b6-5
InchiKey: UWWWGFJWQKVPGQ-AATRIKPKSA-N
Formula: C12H22O2
SMILES: CCC=CCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-105.98	kJ/mol	Joback Method
hf	-423.87	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.322		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
tb	553.97	K	Joback Method
tc	733.78	K	Joback Method
tf	277.08	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.03	J/mol×K	553.97	Joback Method
cpg	517.63	J/mol×K	703.81	Joback Method
cpg	504.62	J/mol×K	673.84	Joback Method
cpg	490.97	J/mol×K	643.87	Joback Method
cpg	476.67	J/mol×K	613.91	Joback Method
cpg	461.70	J/mol×K	583.94	Joback Method
cpg	530.02	J/mol×K	733.78	Joback Method
dvisc	0.0001497	Pa×s	553.97	Joback Method
dvisc	0.0002019	Pa×s	507.82	Joback Method
dvisc	0.0002890	Pa×s	461.67	Joback Method

dvisc	0.0004480	Pa×s	415.52	Joback Method
dvisc	0.0007750	Pa×s	369.38	Joback Method
dvisc	0.0015677	Pa×s	323.23	Joback Method
dvisc	0.0040101	Pa×s	277.08	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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