

(E)-3-hexenyl (Z)-3-hexenoate

Inchi:	InChI=1S/C12H20O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h5-8H,3-4,9-11H2,1-2H3/b7-5+
InchiKey:	UZJQQWFHPLYECS-YMBWGVAGSA-N
Formula:	C12H20O2
SMILES:	CCC=CCCOC(=O)CC=CCC
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
gf	-23.32	kJ/mol	Joback Method
hf	-301.37	kJ/mol	Joback Method
hfus	30.03	kJ/mol	Joback Method
hvap	51.38	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.242		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
ripol	1681.00		NIST Webbook
tb	558.57	K	Joback Method
tc	742.19	K	Joback Method
tf	287.00	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.05	J/mol×K	558.57	Joback Method
cpg	494.87	J/mol×K	711.59	Joback Method
cpg	482.61	J/mol×K	680.98	Joback Method
cpg	469.73	J/mol×K	650.38	Joback Method
cpg	456.20	J/mol×K	619.78	Joback Method
cpg	441.98	J/mol×K	589.17	Joback Method
cpg	506.52	J/mol×K	742.19	Joback Method
dvisc	0.0001355	Pa×s	558.57	Joback Method
dvisc	0.0001789	Pa×s	513.31	Joback Method

dvisc	0.0002493	Pa×s	468.05	Joback Method
dvisc	0.0003730	Pa×s	422.79	Joback Method
dvisc	0.0006146	Pa×s	377.52	Joback Method
dvisc	0.0011604	Pa×s	332.26	Joback Method
dvisc	0.0026769	Pa×s	287.00	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R320895&Units=SI

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

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