(Z)-3-hexenyl 5-hexenoate

Inchi: InChI=1S/C12H20O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h4-5,7H,2-3,6,8-11H2,1H3/b7-5
InchiKey: LKAMWBVFZDHJBB-ALCCZGGFSA-N
Formula: C12H20O2
SMILES: C=CCCCC(=O)OCCC=CCC
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-15.70	kJ/mol	Joback Method
hf	-293.16	kJ/mol	Joback Method
hfus	28.55	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.242		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
ripol	1684.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1686.00		NIST Webbook
tb	551.09	K	Joback Method
tc	730.69	K	Joback Method
tf	290.32	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.90	J/mol×K	551.09	Joback Method
cpg	493.33	J/mol×K	700.76	Joback Method
cpg	481.10	J/mol×K	670.82	Joback Method
cpg	468.27	J/mol×K	640.89	Joback Method
cpg	454.80	J/mol×K	610.96	Joback Method
cpg	440.69	J/mol×K	581.02	Joback Method

cpg	504.97	J/mol×K	730.69	Joback Method
dvisc	0.0001640	Pa×s	551.09	Joback Method
dvisc	0.0002142	Pa×s	507.63	Joback Method
dvisc	0.0002941	Pa×s	464.17	Joback Method
dvisc	0.0004313	Pa×s	420.71	Joback Method
dvisc	0.0006907	Pa×s	377.24	Joback Method
dvisc	0.0012505	Pa×s	333.78	Joback Method
dvisc	0.0027044	Pa×s	290.32	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R313743&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.