

5-hexenyl 5-hexenoate

Inchi:	InChI=1S/C12H20O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h3-4H,1-2,5-11H2
InchiKey:	OQOPHLYZOBOPPA-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	C=CCCCCOC(=O)CCCC=C
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
gf	-8.08	kJ/mol	Joback Method
hf	-284.95	kJ/mol	Joback Method
hfus	27.06	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.242		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
tb	543.61	K	Joback Method
tc	719.25	K	Joback Method
tf	293.64	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.71	J/mol×K	543.61	Joback Method
cpg	491.71	J/mol×K	689.98	Joback Method
cpg	479.51	J/mol×K	660.71	Joback Method
cpg	466.73	J/mol×K	631.43	Joback Method
cpg	453.34	J/mol×K	602.16	Joback Method
cpg	439.34	J/mol×K	572.88	Joback Method
cpg	503.34	J/mol×K	719.25	Joback Method
dvisc	0.0001982	Pa×s	543.61	Joback Method
dvisc	0.0002561	Pa×s	501.95	Joback Method
dvisc	0.0003467	Pa×s	460.29	Joback Method

dvisc	0.0004983	Pa×s	418.62	Joback Method
dvisc	0.0007761	Pa×s	376.96	Joback Method
dvisc	0.0013495	Pa×s	335.30	Joback Method
dvisc	0.0027454	Pa×s	293.64	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=R313609&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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