

2-Hexenoic acid, 2-hexenyl ester, (E,E)-

Other names:	(E)-2-hexenyl (E)-2-hexenoate
Inchi:	InChI=1S/C12H20O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h7-10H,3-6,11H2,1-2H3/b9-7+,
InchiKey:	QZZVRWSUQQJJOS-FIFLTTCUSA-N
Formula:	C12H20O2
SMILES:	CCCC=CCOC(=O)C=CCCC
Mol. weight [g/mol]:	196.29
CAS:	54845-28-2

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	1805.00		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/molxK	558.57	Joback Method
cpg	441.98	J/molxK	589.17	Joback Method
cpg	456.20	J/molxK	619.78	Joback Method
cpg	469.73	J/molxK	650.38	Joback Method
cpg	482.61	J/molxK	680.98	Joback Method
cpg	494.87	J/molxK	711.59	Joback Method
cpg	506.52	J/molxK	742.19	Joback Method

dvisc	0.0026769	Paxs	287.00	Joback Method
dvisc	0.0011604	Paxs	332.26	Joback Method
dvisc	0.0006146	Paxs	377.52	Joback Method
dvisc	0.0003730	Paxs	422.79	Joback Method
dvisc	0.0002493	Paxs	468.05	Joback Method
dvisc	0.0001789	Paxs	513.31	Joback Method
dvisc	0.0001355	Paxs	558.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54845282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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