Heptanoic acid, 3-hexenyl ester, (Z)-

Other names:	(3Z)-3-Hexenyl heptanoate
	cis-3-Hexenyl heptanoate
	(Z)-3-Hexenyl heptanoate
	(Z)-hex-3-enyl heptanoate
Inchi:	InChI=1S/C13H24O2/c1-3-5-7-9-11-13(14)15-12-10-8-6-4-2/h6,8H,3-5,7,9-12H2,1-2H3/b
InchiKey:	KBBLMMCEHYHHIW-VURMDHGXSA-N
Formula:	C13H24O2
SMILES:	CCC=CCCOC(=O)CCCCCC
Mol. weight [g/mol]:	212.33
CAS:	61444-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-95.12	kJ/mol	Joback Method
hf	-439.23	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	53.65	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.856		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1459.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1462.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1730.00		NIST Webbook
tb	577.29	K	Joback Method
tc	752.37	K	Joback Method
tf	303.35	K	Joback Method

vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.80	J/mol×K	577.29	Joback Method
cpg	568.82	J/mol×K	723.19	Joback Method
cpg	555.52	J/mol×K	694.01	Joback Method
cpg	541.59	J/mol×K	664.83	Joback Method
cpg	527.01	J/mol×K	635.65	Joback Method
cpg	511.75	J/mol×K	606.47	Joback Method
cpg	581.49	J/mol×K	752.37	Joback Method
dvisc	0.0001450	Pa×s	577.29	Joback Method
dvisc	0.0001917	Pa×s	531.63	Joback Method
dvisc	0.0002673	Pa×s	485.98	Joback Method
dvisc	0.0003991	Pa×s	440.32	Joback Method
dvisc	0.0006538	Pa×s	394.66	Joback Method
dvisc	0.0012188	Pa×s	349.01	Joback Method
dvisc	0.0027407	Pa×s	303.35	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=C61444391&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume