

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

Other names:	trans-2-Hexenyl caproate trans-2-Hexenyl hexanoate trans-2-Hexenyl n-hexanoate (2E)-2-Hexenyl hexanoate (E)-2-Hexenyl hexanoate (E)-2-Hexenyl n-hexanoate (E)hex-2-enyl hexanoate
Inchi:	InChI=1S/C12H22O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h7,9H,3-6,8,10-11H2,1-2H3/b9
InchiKey:	UQPLEMTXCSYMEK-VQHVLOKHSA-N
Formula:	C12H22O2
SMILES:	CCCC=CCOC(=O)CCCCC
Mol. weight [g/mol]:	198.30
CAS:	53398-86-0

Physical Properties

Property code	Value	Unit	Source
gf	-103.54	kJ/mol	Joback Method
hf	-418.59	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1337.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1368.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1667.00		NIST Webbook

ripol	1656.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1660.00		NIST Webbook
tb	554.41	K	Joback Method
tc	730.90	K	Joback Method
tf	292.08	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.74	J/mol×K	554.41	Joback Method
cpg	461.06	J/mol×K	583.82	Joback Method
cpg	475.72	J/mol×K	613.24	Joback Method
cpg	489.74	J/mol×K	642.65	Joback Method
cpg	503.13	J/mol×K	672.07	Joback Method
cpg	515.92	J/mol×K	701.48	Joback Method
cpg	528.11	J/mol×K	730.90	Joback Method
dvisc	0.0028734	Pa×s	292.08	Joback Method
dvisc	0.0012967	Pa×s	335.80	Joback Method
dvisc	0.0007029	Pa×s	379.52	Joback Method
dvisc	0.0004324	Pa×s	423.25	Joback Method
dvisc	0.0002914	Pa×s	466.97	Joback Method
dvisc	0.0002101	Pa×s	510.69	Joback Method
dvisc	0.0001595	Pa×s	554.41	Joback Method

Sources

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=C53398860&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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