2-Butenoic acid, 3-hexenyl ester, (E,Z)-

Other names:	(3Z)-3-Hexenyl (2E)-2-butenoate
	(Z)-3-Hexenyl (E)-2-butenoate
	2-Butenoic acid, (3Z)-3-hexen-1-yl ester, (2E)-
	(Z)-3-hexenyl crotonate
Inchi:	InChI=1S/C10H16O2/c1-3-5-6-7-9-12-10(11)8-4-2/h4-6,8H,3,7,9H2,1-2H3/b6-5-,8-4-
InchiKey:	KITGYVIOYOCIIE-QUXRQYFZSA-N
Formula:	C10H16O2
SMILES:	CC=CC(=O)OCCC=CCC
Mol. weight [g/mol]:	168.23
CAS:	65405-80-3

Physical Properties

Property code	Value	Unit	Source
gf	-40.16	kJ/mol	Joback Method
hf	-260.09	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	46.93	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.462		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
ripol	1591.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1610.00		NIST Webbook
tb	512.81	K	Joback Method
tc	700.55	K	Joback Method
tf	264.46	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.12	J/mol×K	512.81	Joback Method
cpg	346.55	J/mol×K	544.10	Joback Method
cpg	359.32	J/mol×K	575.39	Joback Method
cpg	371.48	J/mol×K	606.68	Joback Method
cpg	383.03	J/mol×K	637.97	Joback Method
cpg	394.01	J/mol×K	669.26	Joback Method
cpg	404.45	J/mol×K	700.55	Joback Method
dvisc	0.0028273	Pa×s	264.46	Joback Method
dvisc	0.0012643	Pa×s	305.85	Joback Method
dvisc	0.0006849	Pa×s	347.24	Joback Method
dvisc	0.0004228	Pa×s	388.63	Joback Method
dvisc	0.0002864	Pa×s	430.03	Joback Method
dvisc	0.0002077	Pa×s	471.42	Joback Method
dvisc	0.0001587	Pa×s	512.81	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=C65405803&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume