cis-3-Hexenyl iso-butyrate

Other names:	Propanoic acid, 2-methyl-, 3-hexenyl ester, (Z)-
	ENT 33348
	«beta»,«gamma»-Hexenyl isobutanoate
	(Z)-3-hexenyl 2-methylpropanoate
	cis-3-Hexenyl 2-methylbutyrate
	(Z)-3-Hexenyl isobutanoate
	(Z)-Hex-3-enyl isobutyrate
	(Z)-Hex-3-en-1-yl isobutyrate
Inchi:	InChI=1S/C10H18O2/c1-4-5-6-7-8-12-10(11)9(2)3/h5-6,9H,4,7-8H2,1-3H3/b6-5-
InchiKey:	OSMAJVWUIUORGC-WAYWQWQTSA-N
Formula:	C10H18O2
SMILES:	CCC=CCCOC(=O)C(C)C
Mol. weight [g/mol]:	170.25
CAS:	41519-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-122.82	kJ/mol	Joback Method
hf	-382.59	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	46.58	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1145.30		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1145.30		NIST Webbook
rinpol	1145.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1482.00		NIST Webbook
tb	508.21	K	Joback Method
tc	691.70	K	Joback Method
tf	254.54	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.97	J/mol×K	508.21	Joback Method
cpg	365.14	J/mol×K	538.79	Joback Method
cpg	378.69	J/mol×K	569.37	Joback Method
cpg	391.64	J/mol×K	599.96	Joback Method
cpg	404.00	J/mol×K	630.54	Joback Method
cpg	415.79	J/mol×K	661.12	Joback Method
cpg	427.02	J/mol×K	691.70	Joback Method
dvisc	0.0043796	Pa×s	254.54	Joback Method
dvisc	0.0017548	Pa×s	296.82	Joback Method
dvisc	0.0008832	Pa×s	339.10	Joback Method
dvisc	0.0005176	Pa×s	381.38	Joback Method
dvisc	0.0003375	Pa×s	423.65	Joback Method
dvisc	0.0002378	Pa×s	465.93	Joback Method
dvisc	0.0001776	Pa×s	508.21	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41519237&Units=SI
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

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