3-Hexenyl 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-AATRIKPKSA-N
Formula: C10H18O2
SMILES: CCC=CCCOC(=O)C(C)C
Mol. weight [g/mol]: 170.25
CAS: 57859-47-9

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
ripol	1504.00		NIST Webbook
ripol	1504.00		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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57305e+01
Coeff. B	-4.51965e+03
Coeff. C	-7.63250e+01
Temperature range (K), min.	368.99
Temperature range (K), max.	510.11

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R234729&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume