(E)-2-Hexenyl isobutyrate

Inchi: InChI=1S/C10H18O2/c1-4-5-6-7-8-12-10(11)9(2)3/h6-7,9H,4-5,8H2,1-3H3/b7-6+
InchiKey: DSFNTAVCWZDPEB-VOTSOKGWSA-N
Formula: C10H18O2
SMILES: CCCC=CCOC(=O)C(C)C
Mol. weight [g/mol]: 170.25

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	1152.00		NIST Webbook
ripol	1393.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1390.00		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	415.79	J/mol×K	661.12	Joback Method
cpg	404.00	J/mol×K	630.54	Joback Method
cpg	391.64	J/mol×K	599.96	Joback Method
cpg	378.69	J/mol×K	569.37	Joback Method

cpg	365.14	J/mol×K	538.79	Joback Method
cpg	427.02	J/mol×K	691.70	Joback Method
dvisc	0.0001776	Pa×s	508.21	Joback Method
dvisc	0.0002378	Pa×s	465.93	Joback Method
dvisc	0.0003375	Pa×s	423.65	Joback Method
dvisc	0.0005176	Pa×s	381.38	Joback Method
dvisc	0.0008832	Pa×s	339.10	Joback Method
dvisc	0.0017548	Pa×s	296.82	Joback Method
dvisc	0.0043796	Pa×s	254.54	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=R196746&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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