(Z)-3-Hexenyl 2-methylbutyrate

Inchi: InChI=1S/C11H20O2/c1-4-6-7-8-9-13-11(12)10(3)5-2/h7-8,10H,4-6,9H2,1-3H3/b8-7-
InchiKey: SXJKRFLZGRFPBD-FPLPWBNLSA-N
Formula: C11H20O2
SMILES: CCCC=CCOC(=O)C(C)CC
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-114.40	kJ/mol	Joback Method
hf	-403.23	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.932		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1219.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1219.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1463.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1448.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1463.00		NIST Webbook
tb	531.09	K	Joback Method
tc	712.68	K	Joback Method
tf	265.81	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.61	J/mol×K	531.09	Joback Method
cpg	412.58	J/mol×K	561.36	Joback Method
cpg	426.88	J/mol×K	591.62	Joback Method
cpg	440.55	J/mol×K	621.89	Joback Method
cpg	453.60	J/mol×K	652.15	Joback Method
cpg	466.04	J/mol×K	682.42	Joback Method
cpg	477.89	J/mol×K	712.68	Joback Method
dvisc	0.0042170	Pa×s	265.81	Joback Method
dvisc	0.0016682	Pa×s	310.02	Joback Method
dvisc	0.0008318	Pa×s	354.24	Joback Method
dvisc	0.0004840	Pa×s	398.45	Joback Method
dvisc	0.0003138	Pa×s	442.66	Joback Method
dvisc	0.0002201	Pa×s	486.88	Joback Method
dvisc	0.0001638	Pa×s	531.09	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=R196800&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
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