Butanoic acid, 3-methyl-, 2-hexenyl ester, (E)-

Other names: (E)-2-Hexenyl 3-methylbutyrate
Inchi: InChI=1S/C11H20O2/c1-4-5-6-7-8-13-11(12)9-10(2)3/h6-7,10H,4-5,8-9H2,1-3H3/b7-6+
InchiKey: SAVRWHQEMHIAEB-VOTSOKGWSA-N
Formula: C11H20O2
SMILES: CCCC=CCOC(=O)CC(C)C
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	1245.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1490.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U131828&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