2-Hexenyl butanoate, isomer # 1

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

Physical Properties

Property code	Value	Unit	Source
gf	-120.38	kJ/mol	Joback Method
hf	-377.31	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	46.97	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.686		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
ripol	1896.00		NIST Webbook
tb	508.65	K	Joback Method
tc	688.43	K	Joback Method
tf	269.54	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.74	J/mol×K	508.65	Joback Method
cpg	414.10	J/mol×K	658.47	Joback Method
cpg	402.54	J/mol×K	628.50	Joback Method
cpg	390.44	J/mol×K	598.54	Joback Method
cpg	377.79	J/mol×K	568.58	Joback Method
cpg	364.56	J/mol×K	538.61	Joback Method
cpg	425.13	J/mol×K	688.43	Joback Method
dvisc	0.0001880	Pa×s	508.65	Joback Method
dvisc	0.0002455	Pa×s	468.80	Joback Method

dvisc	0.0003369	Pa×s	428.95	Joback Method
dvisc	0.0004933	Pa×s	389.10	Joback Method
dvisc	0.0007878	Pa×s	349.24	Joback Method
dvisc	0.0014196	Pa×s	309.39	Joback Method
dvisc	0.0030444	Pa×s	269.54	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=R518720&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume