3-Hexenoic acid, butyl ester, (Z)-

Other names:	Butyl (Z)-3-hexenoate
Inchi:	InChI=1S/C10H18O2/c1-3-5-7-8-10(11)12-9-6-4-2/h5,7H,3-4,6,8-9H2,1-2H3/b7-5-
InchiKey:	XZKZOAYDHBSAQW-ALCCZGGFSA-N
Formula:	C10H18O2
SMILES:	CCC=CCC(=O)OCCCC
Mol. weight [g/mol]:	170.25
CAS:	69668-84-4

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	1421.00		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	364.56	J/mol×K	538.61	Joback Method
cpg	377.79	J/mol×K	568.58	Joback Method
cpg	390.44	J/mol×K	598.54	Joback Method
cpg	402.54	J/mol×K	628.50	Joback Method
cpg	414.10	J/mol×K	658.47	Joback Method
cpg	425.13	J/mol×K	688.43	Joback Method

dvisc	0.0030444	Pa×s	269.54	Joback Method
dvisc	0.0014196	Pa×s	309.39	Joback Method
dvisc	0.0007878	Pa×s	349.24	Joback Method
dvisc	0.0004933	Pa×s	389.10	Joback Method
dvisc	0.0003369	Pa×s	428.95	Joback Method
dvisc	0.0002455	Pa×s	468.80	Joback Method
dvisc	0.0001880	Pa×s	508.65	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=C69668844&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

Latest version available from:
https://www.chemeo.com/cid/90-963-3/3-Hexenoic-acid-butyl-ester-Z.pdf
Generated by Cheméo on 2024-10-12 07:21:24.699794312 +0000 UTC m=+3298547.336763559.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.