Butanoic acid, 5-hexenyl ester

Other names: 5-Hexenyl butyrate
Inchi: InChI=1S/C10H18O2/c1-3-5-6-7-9-12-10(11)8-4-2/h3H,1,4-9H2,2H3
InchiKey: YLSXHHJLLXESHB-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: C=CCCCCOC(=O)CCC
Mol. weight [g/mol]: 170.25
CAS: 108058-75-9

Physical Properties

Property code	Value	Unit	Source
gf	-112.76	kJ/mol	Joback Method
hf	-369.10	kJ/mol	Joback Method
hfus	23.16	kJ/mol	Joback Method
hvap	46.34	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.686		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1183.00		NIST Webbook
rinpol	1183.00		NIST Webbook
ripol	1456.00		NIST Webbook
ripol	1462.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1456.00		NIST Webbook
ripol	1462.00		NIST Webbook
tb	501.17	K	Joback Method
tc	676.68	K	Joback Method
tf	272.86	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	349.85	J/mol×K	501.17	Joback Method
cpg	363.46	J/mol×K	530.42	Joback Method
cpg	376.52	J/mol×K	559.67	Joback Method
cpg	389.06	J/mol×K	588.93	Joback Method
cpg	401.07	J/mol×K	618.18	Joback Method
cpg	412.57	J/mol×K	647.43	Joback Method
cpg	423.57	J/mol×K	676.68	Joback Method
dvisc	0.0030420	Pa×s	272.86	Joback Method
dvisc	0.0015143	Pa×s	310.91	Joback Method
dvisc	0.0008777	Pa×s	348.96	Joback Method
dvisc	0.0005663	Pa×s	387.01	Joback Method
dvisc	0.0003952	Pa×s	425.07	Joback Method
dvisc	0.0002926	Pa×s	463.12	Joback Method
dvisc	0.0002268	Pa×s	501.17	Joback Method

Sources

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=C108058759&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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