Hexanoic acid, 5-hexenyl ester

Other names: 5-hexenyl hexanoate
Inchi: InChI=1S/C12H22O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h3H,1,4-11H2,2H3
InchiKey: LTHBRQQXKACRAP-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: C=CCCCCOC(=O)CCCCC
Mol. weight [g/mol]: 198.30
CAS: 108058-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-95.92	kJ/mol	Joback Method
hf	-410.38	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	50.79	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
ripol	1652.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1652.00		NIST Webbook
tb	546.93	K	Joback Method
tc	719.58	K	Joback Method
tf	295.40	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.34	J/mol×K	546.93	Joback Method
cpg	459.51	J/mol×K	575.71	Joback Method
cpg	474.05	J/mol×K	604.48	Joback Method
cpg	487.98	J/mol×K	633.26	Joback Method

cpg	501.31	J/mol×K	662.03	Joback Method
cpg	514.06	J/mol×K	690.81	Joback Method
cpg	526.24	J/mol×K	719.58	Joback Method
dvisc	0.0029144	Pa×s	295.40	Joback Method
dvisc	0.0013996	Pa×s	337.32	Joback Method
dvisc	0.0007904	Pa×s	379.24	Joback Method
dvisc	0.0005002	Pa×s	421.17	Joback Method
dvisc	0.0003439	Pa×s	463.09	Joback Method
dvisc	0.0002516	Pa×s	505.01	Joback Method
dvisc	0.0001931	Pa×s	546.93	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=C108058817&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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