Hexyl 3-butenoate

Other names: 3-Butenoic acid, hexyl ester
Inchi: InChI=1S/C10H18O2/c1-3-5-6-7-9-12-10(11)8-4-2/h4H,2-3,5-9H2,1H3
InchiKey: NSYNOHXVZCEBTM-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: C=CCC(=O)OCCCCCC
Mol. weight [g/mol]: 170.25

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	1142.00		NIST Webbook
rinpol	1160.00		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=R5331&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume