(Z)-hex-3-enyl (Z)-hex-3-enoate

Other names: (Z)-(Z)-Hex-3-en-1-yl hex-3-enoate
Inchi: InChI=1S/C12H20O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h5-8H,3-4,9-11H2,1-2H3/b7-5-,
InchiKey: UZJQQWFHPLYECS-SFECMWDFSA-N
Formula: C12H20O2
SMILES: CCC=CCCOC(=O)CC=CCC
Mol. weight [g/mol]: 196.29
CAS: 61444-38-0

Physical Properties

Property code	Value	Unit	Source
gf	-23.32	kJ/mol	Joback Method
hf	-301.37	kJ/mol	Joback Method
hfus	30.03	kJ/mol	Joback Method
hvap	51.38	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.242		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1388.80		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1715.00		NIST Webbook
ripol	1715.00		NIST Webbook
tb	558.57	K	Joback Method
tc	742.19	K	Joback Method
tf	287.00	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.05	J/mol×K	558.57	Joback Method
cpg	441.98	J/mol×K	589.17	Joback Method
cpg	456.20	J/mol×K	619.78	Joback Method
cpg	469.73	J/mol×K	650.38	Joback Method

cpg	482.61	J/mol×K	680.98	Joback Method
cpg	494.87	J/mol×K	711.59	Joback Method
cpg	506.52	J/mol×K	742.19	Joback Method
dvisc	0.0026769	Pa×s	287.00	Joback Method
dvisc	0.0011604	Pa×s	332.26	Joback Method
dvisc	0.0006146	Pa×s	377.52	Joback Method
dvisc	0.0003730	Pa×s	422.79	Joback Method
dvisc	0.0002493	Pa×s	468.05	Joback Method
dvisc	0.0001789	Pa×s	513.31	Joback Method
dvisc	0.0001355	Pa×s	558.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61444380&Units=SI
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

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