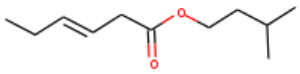
3-hexenyl-3-methylbutanoate

Other names: hex-3-enyl isovalerate.
InChI: InChI=1S/C11H20O2/c1-4-5-6-7-11(12)13-9-8-10(2)3/h5-6,10H,4,7-9H2,1-3H3/b6-5+
InChI Key: NKKNXGRSBVQXTN-AATRIKPKSA-N
Formula: C11H20O2
SMILES: CCC=CCC(=O)OCCC(C)C
Molecular Weight: 184.28
CAS: 10032-11-8



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-114.40	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-403.23	kJ/mol	Joback Method
$\Delta_{fus} H°$	23.71	kJ/mol	Joback Method
$\Delta_{vap} H°$	48.81	kJ/mol	Joback Method
$logP_{oct/wat}$	2.93		Crippen Method
P_c	2127.56	kPa	Joback Method
T_{boil}	531.09	K	Joback Method
T_c	712.68	K	Joback Method
T_{fus}	265.81	K	Joback Method
V_c	0.65	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	397.61	J/mol×K	531.09	Joback Method
η	0.00	Pa×s	531.09	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H20O2/c1-4-5-6-7-11(12)13-9-8-10(2)3/h5-6,10H,4,7-9H2,1-3H3/b6-5+
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).