Hexanoic acid, 3-methyl-2-butenyl ester

Other names: Hexanoic acid, 3-methylbut-2-enyl ester
3-methyl-2-butenyl hexanoate
3-methylbut-2-enyl hexanoate
Inchi: InChI=1S/C11H20O2/c1-4-5-6-7-11(12)13-9-8-10(2)3/h8H,4-7,9H2,1-3H3
InchiKey: MUVXQQVJNUBWPF-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: CCCCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 184.28
CAS: 76649-22-4

Physical Properties

Property code	Value	Unit	Source
gf	-120.51	kJ/mol	Joback Method
hf	-407.74	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	49.27	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1284.00		NIST Webbook
rinpol	1244.00		NIST Webbook
ripol	1572.00		NIST Webbook
tb	531.41	K	Joback Method
tc	712.45	K	Joback Method
tf	266.85	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.17	J/mol×K	531.41	Joback Method
cpg	412.00	J/mol×K	561.58	Joback Method
cpg	426.18	J/mol×K	591.76	Joback Method

cpg	439.73	J/mol×K	621.93	Joback Method
cpg	452.68	J/mol×K	652.10	Joback Method
cpg	465.03	J/mol×K	682.28	Joback Method
cpg	476.80	J/mol×K	712.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76649224&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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