3-methyl-3-butenyl hexanoate

Inchi: InChI=1S/C11H20O2/c1-4-5-6-7-11(12)13-9-8-10(2)3/h2,4-9H2,1,3H3
InchiKey: PFKCNOUVNPEGIF-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: C=C(C)CCOC(=O)CCCCC
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-112.89	kJ/mol	Joback Method
hf	-399.53	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	48.65	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1213.00		NIST Webbook
ripol	1522.00		NIST Webbook
tb	523.93	K	Joback Method
tc	700.83	K	Joback Method
tf	270.17	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.02	J/mol×K	523.93	Joback Method
cpg	410.66	J/mol×K	553.41	Joback Method
cpg	424.70	J/mol×K	582.90	Joback Method
cpg	438.14	J/mol×K	612.38	Joback Method
cpg	451.01	J/mol×K	641.86	Joback Method
cpg	463.32	J/mol×K	671.35	Joback Method

cpg	475.06	J/mol×K	700.83	Joback Method

Sources

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=R238083&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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