(Z,Z)-3-hexenyl 2-methyl-2-butenoate

Other names: (Z)-(Z)-Hex-3-en-1-yl 2-methylbut-2-enoate
Inchi: InChI=1S/C11H18O2/c1-4-6-7-8-9-13-11(12)10(3)5-2/h5-7H,4,8-9H2,1-3H3/b7-6-,10-5-
InchiKey: JNWQKXUWZWKUAY-BHHIIOOYSA-N
Formula: C11H18O2
SMILES: CC=C(C)C(=O)OCCC=CCC
Mol. weight [g/mol]: 182.26
CAS: 84060-80-0

Physical Properties

Property code	Value	Unit	Source
gf	-40.29	kJ/mol	Joback Method
hf	-290.52	kJ/mol	Joback Method
hfus	26.13	kJ/mol	Joback Method
hvap	49.23	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.852		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1282.20		NIST Webbook
tb	535.57	K	Joback Method
tc	724.37	K	Joback Method
tf	261.77	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.03	J/mol×K	535.57	Joback Method
cpg	393.47	J/mol×K	567.04	Joback Method
cpg	407.20	J/mol×K	598.50	Joback Method
cpg	420.25	J/mol×K	629.97	Joback Method
cpg	432.66	J/mol×K	661.44	Joback Method
cpg	444.45	J/mol×K	692.91	Joback Method
cpg	455.65	J/mol×K	724.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84060800&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume