Hex-3-enyl 2-methylbutanoate

Other names: 3-hexenyl-2-methylbutanoate
Inchi: InChI=1S/C11H20O2/c1-4-6-7-8-9-13-11(12)10(3)5-2/h6-7,10H,4-5,8-9H2,1-3H3/b7-6-
InchiKey: JKKGTSUICJWEKB-SREVYHEPSA-N
Formula: C11H20O2
SMILES: CCC=CCCOC(=O)C(C)CC
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-114.40	kJ/mol	Joback Method
hf	-403.23	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.932		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1254.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1224.00		NIST Webbook
tb	531.09	K	Joback Method
tc	712.68	K	Joback Method
tf	265.81	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.61	J/mol×K	531.09	Joback Method
cpg	412.58	J/mol×K	561.36	Joback Method
cpg	426.88	J/mol×K	591.62	Joback Method
cpg	440.55	J/mol×K	621.89	Joback Method

cpg	453.60	J/mol×K	652.15	Joback Method
cpg	466.04	J/mol×K	682.42	Joback Method
cpg	477.89	J/mol×K	712.68	Joback Method
dvisc	0.0042170	Pa×s	265.81	Joback Method
dvisc	0.0016682	Pa×s	310.02	Joback Method
dvisc	0.0008318	Pa×s	354.24	Joback Method
dvisc	0.0004840	Pa×s	398.45	Joback Method
dvisc	0.0003138	Pa×s	442.66	Joback Method
dvisc	0.0002201	Pa×s	486.88	Joback Method
dvisc	0.0001638	Pa×s	531.09	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=R231433&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume