Hexyl tiglate

Other names:	hexyl 2-methyl-2-butenoate
	hexyl crotonate
Inchi:	InChI=1S/C11H20O2/c1-4-6-7-8-9-13-11(12)10(3)5-2/h5H,4,6-9H2,1-3H3/b10-5+
InchiKey:	JTCIUOKKVACNCK-BJMVGYQFSA-N
Formula:	C11H20O2
SMILES:	CC=C(C)C(=O)OCCCCCC
Mol. weight [g/mol]:	184.28
CAS:	16930-96-4

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	1310.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1333.40		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1316.00		NIST Webbook

rinpol	1333.40		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1622.00		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

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=C16930964&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