(E)-2-Hexenyl tiglate

Other names: trans-2-Hexenyl tiglate
Inchi: InChI=1S/C11H18O2/c1-4-6-7-8-9-13-11(12)10(3)5-2/h5,7-8H,4,6,9H2,1-3H3/b8-7+,10-5
InchiKey: UEDNMMNLPZRYMI-LZIZUESTSA-N
Formula: C11H18O2
SMILES: CC=C(C)C(=O)OCC=CCCC
Mol. weight [g/mol]: 182.26

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	1340.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1338.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1672.00		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

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U131836&Units=SI

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