Ionyl tiglate, methyl-«beta»-(E)-

Other names: Methyl-«beta»-(E)-ionyl tiglate
Inchi: InChI=1S/C19H30O2/c1-8-13(2)18(20)21-16(5)15(4)12-17-14(3)10-9-11-19(17,6)7/h8,12
InchiKey: KPRKGDYBUQYSOZ-MKRNSSSCSA-N
Formula: C19H30O2
SMILES: CC=C(C)C(=O)OC(C)C(C)=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	45.74	kJ/mol	Joback Method
hf	-366.31	kJ/mol	Joback Method
hfus	28.00	kJ/mol	Joback Method
hvap	67.63	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.357		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
ripol	2185.00		NIST Webbook
ripol	2185.00		NIST Webbook
tb	746.96	K	Joback Method
tc	961.88	K	Joback Method
tf	380.05	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.16	J/mol×K	746.96	Joback Method
cpg	789.60	J/mol×K	782.78	Joback Method
cpg	809.21	J/mol×K	818.60	Joback Method
cpg	828.14	J/mol×K	854.42	Joback Method
cpg	846.52	J/mol×K	890.24	Joback Method
cpg	864.50	J/mol×K	926.06	Joback Method
cpg	882.21	J/mol×K	961.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383629&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume