Pseudoisoeugenyl tiglate

Inchi: InChI=1S/C15H18O3/c1-5-7-12-8-9-13(14(10-12)17-4)18-15(16)11(3)6-2/h5-10H,1-4H3/
InchiKey: ZTMOFQLUZSNPJG-UHYUDDSYSA-N
Formula: C15H18O3
SMILES: CC=Cc1ccc(OC(=O)C(C)=CC)c(OC)c1
Mol. weight [g/mol]: 246.30

Physical Properties

Property code	Value	Unit	Source
gf	-18.46	kJ/mol	Joback Method
hf	-291.71	kJ/mol	Joback Method
hfus	30.94	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.600		Crippen Method
mcvol	203.160	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1818.00		NIST Webbook
tb	686.15	K	Joback Method
tc	901.85	K	Joback Method
tf	380.54	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.20	J/mol×K	686.15	Joback Method
cpg	543.49	J/mol×K	722.10	Joback Method
cpg	557.86	J/mol×K	758.05	Joback Method
cpg	571.35	J/mol×K	794.00	Joback Method
cpg	583.98	J/mol×K	829.95	Joback Method
cpg	595.79	J/mol×K	865.90	Joback Method
cpg	606.81	J/mol×K	901.85	Joback Method

Sources

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=R240076&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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