4-(1-Propenyl)-phenyl tiglate

Inchi: InChI=1S/C14H16O2/c1-4-6-12-7-9-13(10-8-12)16-14(15)11(3)5-2/h4-10H,1-3H3/b6-4+,
InchiKey: UCQRFKUYPJOHMR-KGUOMNFLSA-N
Formula: C14H16O2
SMILES: CC=Cc1ccc(OC(=O)C(C)=CC)cc1
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
gf	87.75	kJ/mol	Joback Method
hf	-127.38	kJ/mol	Joback Method
hfus	27.55	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.591		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
ripol	2406.00		NIST Webbook
ripol	2406.00		NIST Webbook
ripol	2406.00		NIST Webbook
tb	635.87	K	Joback Method
tc	857.03	K	Joback Method
tf	334.52	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.35	J/mol×K	635.87	Joback Method
cpg	466.66	J/mol×K	672.73	Joback Method
cpg	481.00	J/mol×K	709.59	Joback Method
cpg	494.40	J/mol×K	746.45	Joback Method
cpg	506.94	J/mol×K	783.31	Joback Method
cpg	518.67	J/mol×K	820.17	Joback Method
cpg	529.64	J/mol×K	857.03	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=R418269&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume