4-(3-Methyloxiranyl)-phenyl tiglate

Inchi: InChI=1S/C14H16O3/c1-4-9(2)14(15)17-12-7-5-11(6-8-12)13-10(3)16-13/h4-8,10,13H,1-
InchiKey: NVVSTEISAGGUMC-RUDMXATFSA-N
Formula: C14H16O3
SMILES: CC=C(C)C(=O)Oc1ccc(C2OC2C)cc1
Mol. weight [g/mol]: 232.28

Physical Properties

Property code	Value	Unit	Source
gf	-25.55	kJ/mol	Joback Method
hf	-324.14	kJ/mol	Joback Method
hfus	34.53	kJ/mol	Joback Method
hvap	63.00	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.018		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
ripol	2642.00		NIST Webbook
ripol	2642.00		NIST Webbook
tb	660.73	K	Joback Method
tc	885.13	K	Joback Method
tf	379.87	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.02	J/mol×K	660.73	Joback Method
cpg	507.03	J/mol×K	698.13	Joback Method
cpg	521.98	J/mol×K	735.53	Joback Method
cpg	535.91	J/mol×K	772.93	Joback Method
cpg	548.91	J/mol×K	810.33	Joback Method
cpg	561.02	J/mol×K	847.73	Joback Method
cpg	572.32	J/mol×K	885.13	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=R418289&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