3-Oxo-«alpha»-ionol, Gly, TFA

Inchi: InChI=1S/C27H28F12O10/c1-11-6-5-9-23(3,4)13(11)8-7-12(2)45-18-17(49-22(43)27(37,
InchiKey: NGUMVGJAUDODIR-FUQKTWFESA-N
Formula: C27H28F12O10
SMILES: CC1=CCCC(C)(C)C1C=CC(C)OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)
Mol. weight [g/mol]: 740.49

Physical Properties

Property code	Value	Unit	Source
gf	-3173.73	kJ/mol	Joback Method
hf	-4051.92	kJ/mol	Joback Method
hfus	73.54	kJ/mol	Joback Method
hvap	102.94	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	5.583		Crippen Method
mcvol	423.710	ml/mol	McGowan Method
pc	713.01	kPa	Joback Method
rinpol	2127.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2127.00		NIST Webbook
tb	1173.86	K	Joback Method
tc	1484.05	K	Joback Method
tf	758.91	K	Joback Method
vc	1.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1597.03	J/mol×K	1173.86	Joback Method
cpg	1617.81	J/mol×K	1225.56	Joback Method
cpg	1638.10	J/mol×K	1277.26	Joback Method
cpg	1658.34	J/mol×K	1328.96	Joback Method
cpg	1678.99	J/mol×K	1380.66	Joback Method
cpg	1700.50	J/mol×K	1432.36	Joback Method
cpg	1723.32	J/mol×K	1484.05	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=R394628&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume