4-Oxo-«beta»-ionol, Gly, TFA

Inchi: InChI=1S/C27H26F12O11/c1-10-7-12(40)8-23(3,4)13(10)6-5-11(2)46-18-17(50-22(44)27
InchiKey: AMGTVCUHNCZYHT-KUPPMWNHSA-N
Formula: C27H26F12O11
SMILES: CC1=C(C=CC(C)OC2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2O
Mol. weight [g/mol]: 754.47

Physical Properties

Property code	Value	Unit	Source
gf	-3298.24	kJ/mol	Joback Method
hf	-4180.75	kJ/mol	Joback Method
hfus	71.59	kJ/mol	Joback Method
hvap	108.16	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	4.906		Crippen Method
mcvol	425.280	ml/mol	McGowan Method
pc	733.63	kPa	Joback Method
rinpol	2220.00		NIST Webbook
tb	1251.33	K	Joback Method
tc	1597.48	K	Joback Method
tf	843.89	K	Joback Method
vc	1.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1606.20	J/mol×K	1251.33	Joback Method
cpg	1623.78	J/mol×K	1309.02	Joback Method
cpg	1640.48	J/mol×K	1366.71	Joback Method
cpg	1656.81	J/mol×K	1424.40	Joback Method
cpg	1673.28	J/mol×K	1482.09	Joback Method
cpg	1690.38	J/mol×K	1539.78	Joback Method
cpg	1708.64	J/mol×K	1597.48	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=R394633&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