Vomifoliol 1A, Gly, TFA

Inchi: InChI=1S/C27H26F12O12/c1-10-7-12(40)8-22(3,4)23(10,45)6-5-11(2)47-17-16(51-21(44
InchiKey: RLAMSVSKZSJPFN-RNPOMOAQSA-N
Formula: C27H26F12O12
SMILES: CC1=CC(=O)CC(C)(C)C1(O)C=CC(C)OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(
Mol. weight [g/mol]: 770.47

Physical Properties

Property code	Value	Unit	Source
gf	-3438.63	kJ/mol	Joback Method
hf	-4326.61	kJ/mol	Joback Method
hfus	70.84	kJ/mol	Joback Method
hvap	122.71	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	3.877		Crippen Method
mcvol	431.150	ml/mol	McGowan Method
pc	783.31	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	1334.10	K	Joback Method
tc	1763.09	K	Joback Method
tf	911.85	K	Joback Method
vc	1.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1757.13	J/mol×K	1334.10	Joback Method
cpg	1813.20	J/mol×K	1405.60	Joback Method
cpg	1876.47	J/mol×K	1477.10	Joback Method
cpg	1948.58	J/mol×K	1548.59	Joback Method
cpg	2031.16	J/mol×K	1620.09	Joback Method
cpg	2125.84	J/mol×K	1691.59	Joback Method
cpg	2234.24	J/mol×K	1763.09	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=R394797&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