

Vomifoliol, rutinoside, TFA

Inchi:	InChI=1S/C38H31F21O19/c1-11(5-7-31(78-29(67)38(57,58)59)8-6-13(60)9-30(31,3)4)69
InchiKey:	DGJXAFGHCBDCBS-HYAJ SXBFSA-N
Formula:	C38H31F21O19
SMILES:	CC(C=CC1(OC(=O)C(F)(F)F)C=CC(=O)CC1(C)C)OC1OC(COC2OC(C)C(OC(=O)C(F)(F)F)C)O2
Mol. weight [g/mol]:	1190.61

Physical Properties

Property code	Value	Unit	Source
gf	-5843.60	kJ/mol	Joback Method
hf	-7206.85	kJ/mol	Joback Method
hfus	114.76	kJ/mol	Joback Method
hvap	152.20	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	5.678		Crippen Method
mvol	619.400	ml/mol	McGowan Method
pc	421.81	kPa	Joback Method
rinpol	2350.00		NIST Webbook
tb	1751.47	K	Joback Method
tc	3314.43	K	Joback Method
tf	1230.75	K	Joback Method
vc	2.463	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2737.63	J/molxK	1751.47	Joback Method
cpg	3102.90	J/molxK	2011.96	Joback Method
cpg	3704.14	J/molxK	2272.46	Joback Method
cpg	4625.90	J/molxK	2532.95	Joback Method
cpg	5952.71	J/molxK	2793.45	Joback Method
cpg	7769.12	J/molxK	3053.94	Joback Method
cpg	10159.66	J/molxK	3314.43	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=R184911&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
mccvol:	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

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