Geraniol, «beta»-D-glycopyranoside, TFA

Other names: Geranyl «beta»-D-glucopyranoside, TFA
Inchi: InChI=1S/C24H24F12O10/c1-10(2)5-4-6-11(3)7-8-41-16-15(46-20(40)24(34,35)36)14(45
InchiKey: UCMHRJFXWFCWDN-PBFODTKESA-N
Formula: C24H24F12O10
SMILES: CC(C)=CCCC(C)=CCOC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F
Mol. weight [g/mol]: 700.42

Physical Properties

Property code	Value	Unit	Source
gf	-3165.01	kJ/mol	Joback Method
hf	-3982.61	kJ/mol	Joback Method
hfus	79.44	kJ/mol	Joback Method
hvap	96.84	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	4.948		Crippen Method
mcvol	392.300	ml/mol	McGowan Method
pc	754.33	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1881.00		NIST Webbook
rinpol	1881.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	1090.32	K	Joback Method
tc	1373.40	K	Joback Method
tf	666.78	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.13	J/mol×K	1090.32	Joback Method
cpg	1404.97	J/mol×K	1137.50	Joback Method
cpg	1413.53	J/mol×K	1184.68	Joback Method
cpg	1420.01	J/mol×K	1231.86	Joback Method
cpg	1424.60	J/mol×K	1279.04	Joback Method

cpg	1427.49	J/mol×K	1326.22	Joback Method
cpg	1428.88	J/mol×K	1373.40	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=R394693&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume