

geranyl 6-O-(«alpha»-L-rhamonopyranosyl)-«beta»-D-glucopyranoside TFA

Other names:	Geraniol, Rut, TFA
Inchi:	InChI=1S/C34H32F18O16/c1-11(2)6-5-7-12(3)8-9-59-21-20(68-28(58)34(50,51)52)18(66
InchiKey:	KRKOLWZUQOBRQW-LKVZFRRBSA-N
Formula:	C34H32F18O16
SMILES:	CC(C)=CCCC(C)=CCOC1OC(COC2OC(C)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2OC
Mol. weight [g/mol]:	1038.58

Physical Properties

Property code	Value	Unit	Source
gf	-4909.34	kJ/mol	Joback Method
hf	-6164.03	kJ/mol	Joback Method
hfus	119.85	kJ/mol	Joback Method
hvap	136.03	kJ/mol	Joback Method
log10ws	-9.16		Crippen Method
logp	6.027		Crippen Method
mcvol	559.580	ml/mol	McGowan Method
pc	453.85	kPa	Joback Method
rinpol	2205.00		NIST Webbook
rinpol	2205.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2205.00		NIST Webbook
tb	1511.10	K	Joback Method
tc	2434.03	K	Joback Method
tf	971.40	K	Joback Method
vc	2.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1996.83	J/mol×K	1511.10	Joback Method
cpg	1923.46	J/mol×K	1664.92	Joback Method
cpg	1827.45	J/mol×K	1818.74	Joback Method
cpg	1715.50	J/mol×K	1972.56	Joback Method
cpg	1594.34	J/mol×K	2126.38	Joback Method

cpg	1470.68	J/mol×K	2280.21	Joback Method
cpg	1351.23	J/mol×K	2434.03	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=R394702&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
hvac:	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

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