

(S)-Linalol rutinoside, TFA

Inchi:	InChI=1S/C34H32F18O16/c1-6-28(5,9-7-8-11(2)3)68-21-19(67-27(58)34(50,51)52)17(65
InchiKey:	GMMCRRIKSGFQIA-AYVOIJCJSA-N
Formula:	C34H32F18O16
SMILES:	C=CC(C)(CCC=C(C)C)OC1OC(COC2OC(C)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2O
Mol. weight [g/mol]:	1038.58

Physical Properties

Property code	Value	Unit	Source
gf	-4890.33	kJ/mol	Joback Method
hf	-6154.78	kJ/mol	Joback Method
hfus	112.26	kJ/mol	Joback Method
hvap	134.03	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	6.025		Crippen Method
mcvol	559.580	ml/mol	McGowan Method
pc	454.63	kPa	Joback Method
rinpol	2130.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	1500.51	K	Joback Method
tc	2374.90	K	Joback Method
tf	991.10	K	Joback Method
vc	2.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2007.14	J/molxK	1500.51	Joback Method
cpg	1946.13	J/molxK	1646.24	Joback Method
cpg	1867.85	J/molxK	1791.97	Joback Method
cpg	1778.77	J/molxK	1937.71	Joback Method
cpg	1685.33	J/molxK	2083.44	Joback Method
cpg	1594.01	J/molxK	2229.17	Joback Method
cpg	1511.24	J/molxK	2374.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R327841&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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