

2-Phenylethanol, rutinoside, TFA

Other names:	Phenethyl alcohol, Rut, TFA
Inchi:	InChI=1S/C32H24F18O16/c1-10-13(61-21(51)27(33,34)35)15(63-23(53)29(39,40)41)17(
InchiKey:	XTZBPLHRZJNARN-PBAYVUIYSA-N
Formula:	C32H24F18O16
SMILES:	CC1OC(OCC2OC(OCCc3ccccc3)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2OC(=O)C(F)(F)F)C1
Mol. weight [g/mol]:	1006.49

Physical Properties

Property code	Value	Unit	Source
gf	-4957.11	kJ/mol	Joback Method
hf	-6101.08	kJ/mol	Joback Method
hfus	110.93	kJ/mol	Joback Method
hvap	133.78	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	4.577		Crippen Method
mcvol	516.240	ml/mol	McGowan Method
pc	544.63	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2201.00		NIST Webbook
tb	1483.94	K	Joback Method
tc	2226.22	K	Joback Method
tf	1013.36	K	Joback Method
vc	2.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1778.49	J/molxK	1483.94	Joback Method
cpg	1696.89	J/molxK	1607.65	Joback Method

cpg	1592.39	J/mol×K	1731.37	Joback Method
cpg	1467.39	J/mol×K	1855.08	Joback Method
cpg	1324.28	J/mol×K	1978.80	Joback Method
cpg	1165.47	J/mol×K	2102.51	Joback Method
cpg	993.33	J/mol×K	2226.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184639&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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