

Benzyl alcohol, rutinose, TFA

Other names:	Benzenemethanol, Rut, TFA benzyl 6- O-(«alpha»-L-rhamonopyranosyl)-«beta»-D-glucopyranoside, TFA
Inchi:	InChI=1S/C31H22F18O16/c1-9-12(60-20(50)26(32,33)34)14(62-22(52)28(38,39)40)16(6
InchiKey:	ZFZXGBPUOBMIRI-FARGQAFFSA-N
Formula:	C31H22F18O16
SMILES:	CC1OC(OCC2OC(OCc3ccccc3)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2OC(=O)C(F)(F)F
Mol. weight [g/mol]:	992.47

Physical Properties

Property code	Value	Unit	Source
gf	-4965.53	kJ/mol	Joback Method
hf	-6080.44	kJ/mol	Joback Method
hfus	108.34	kJ/mol	Joback Method
hvap	131.56	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	4.534		Crippen Method
mcvol	502.150	ml/mol	McGowan Method
pc	569.87	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	1461.06	K	Joback Method
tc	2145.88	K	Joback Method
tf	1002.09	K	Joback Method
vc	2.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1732.00	J/molxK	1461.06	Joback Method

cpg	1660.35	J/mol×K	1575.20	Joback Method
cpg	1568.62	J/mol×K	1689.33	Joback Method
cpg	1458.59	J/mol×K	1803.47	Joback Method
cpg	1332.04	J/mol×K	1917.61	Joback Method
cpg	1190.74	J/mol×K	2031.75	Joback Method
cpg	1036.48	J/mol×K	2145.88	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=R184659&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

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