

Benzenemethanol, Gly, TFA

Other names:	Benzyl alcohol, «beta»-D-glucopyranoside, TFA
Inchi:	InChI=1S/C21H14F12O10/c22-18(23,24)14(34)39-7-9-10(41-15(35)19(25,26)27)11(42-1
InchiKey:	JIMPIJVFGNCEM-WJTVCTBASA-N
Formula:	C21H14F12O10
SMILES:	O=C(OCC1OC(OCc2ccccc2)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F
Mol. weight [g/mol]:	654.31

Physical Properties

Property code	Value	Unit	Source
gf	-3221.20	kJ/mol	Joback Method
hf	-3899.02	kJ/mol	Joback Method
hfus	67.93	kJ/mol	Joback Method
hvap	92.36	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	3.456		Crippen Method
mcvol	334.870	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	1040.28	K	Joback Method
tc	1283.00	K	Joback Method
tf	697.47	K	Joback Method
vc	1.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.42	J/molxK	1040.28	Joback Method
cpg	1170.06	J/molxK	1080.73	Joback Method

cpg	1174.70	J/mol×K	1121.19	Joback Method
cpg	1177.42	J/mol×K	1161.64	Joback Method
cpg	1178.30	J/mol×K	1202.10	Joback Method
cpg	1177.41	J/mol×K	1242.55	Joback Method
cpg	1174.83	J/mol×K	1283.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184644&Units=SI
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

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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