Hexanol «beta»-D-glucopyranoside, TFA

Other names: Hexanol, Gly, TFA
Inchi: InChI=1S/C20H20F12O10/c1-2-3-4-5-6-37-12-11(42-16(36)20(30,31)32)10(41-15(35)19(
InchiKey: WIBWLTPJESIJNR-RMPHRYRLSA-N
Formula: C20H20F12O10
SMILES: CCCCCCOC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C
Mol. weight [g/mol]: 648.35

Physical Properties

Property code	Value	Unit	Source
gf	-3342.03	kJ/mol	Joback Method
hf	-4114.91	kJ/mol	Joback Method
hfus	71.29	kJ/mol	Joback Method
hvap	87.86	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	3.836		Crippen Method
mcvol	344.540	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1640.00		NIST Webbook
tb	990.72	K	Joback Method
tc	1231.77	K	Joback Method
tf	659.78	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.98	J/mol×K	990.72	Joback Method
cpg	1229.82	J/mol×K	1030.89	Joback Method
cpg	1238.49	J/mol×K	1071.07	Joback Method
cpg	1245.07	J/mol×K	1111.24	Joback Method

cpg	1249.60	J/mol×K	1151.42	Joback Method
cpg	1252.16	J/mol×K	1191.59	Joback Method
cpg	1252.80	J/mol×K	1231.77	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=R190699&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
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