benzyl 6-O-(«alpha»-L-arabinofuranosyl)-«beta»-D-glucopy TFA

Other names: Benzenemethanol, «alpha»-L-Arabinofuranosyl-«beta»-D-Glucopyranoside, TFA

Inchi: InChI=1S/C30H20F18O16/c31-25(32,33)19(49)57-8-11-13(61-21(51)27(37,38)39)15(63-

InchiKey: RLAJQRZPNBQZPM-NLBOSZRJSA-N

Formula: C30H20F18O16

SMILES: O=C(OCC1OC(OCC2OC(OCc3ccccc3)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2OC(=O

Mol. weight [g/mol]: 978.44

Physical Properties

Property code	Value	Unit	Source
gf	-4954.14	kJ/mol	Joback Method
hf	-6033.30	kJ/mol	Joback Method
hfus	106.78	kJ/mol	Joback Method
hvap	129.47	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	4.146		Crippen Method
mcvol	488.060	ml/mol	McGowan Method
pc	599.26	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2175.00		NIST Webbook
tb	1438.58	K	Joback Method
tc	2096.23	K	Joback Method
tf	998.58	K	Joback Method
vc	1.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1698.38	J/mol×K	1438.58	Joback Method
cpg	1645.88	J/mol×K	1548.19	Joback Method
cpg	1578.50	J/mol×K	1657.80	Joback Method
cpg	1498.18	J/mol×K	1767.41	Joback Method
cpg	1406.85	J/mol×K	1877.02	Joback Method
cpg	1306.45	J/mol×K	1986.63	Joback Method

cpg	1198.92	J/mol×K	2096.23	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=R394648&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