

Furaneol, «beta»-D-glucopyranoside, TFA

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H14F12O12/c1-4-7(33)8(5(2)39-4)41-12-11(44-16(37)20(30,31)32)10(43-1

RTCLBMVJHDXPSV-MFLT XKOCSA-N

C20H14F12O12

CC1=C(OC2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2OC(=O)C

674.30

Physical Properties

Property code	Value	Unit	Source
gf	-3503.49	kJ/mol	Joback Method
hf	-4289.29	kJ/mol	Joback Method
hfus	73.16	kJ/mol	Joback Method
hvap	98.49	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	2.475		Crippen Method
mcvol	336.820	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	1668.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
tb	1109.89	K	Joback Method
tc	1379.40	K	Joback Method
tf	791.27	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1203.23	J/mol×K	1109.89	Joback Method
cpg	1204.73	J/mol×K	1154.81	Joback Method
cpg	1203.09	J/mol×K	1199.73	Joback Method
cpg	1198.34	J/mol×K	1244.64	Joback Method
cpg	1190.49	J/mol×K	1289.56	Joback Method
cpg	1179.55	J/mol×K	1334.48	Joback Method
cpg	1165.56	J/mol×K	1379.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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