

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-SVNGYHJRSA-N
Formula:	C20H20F12O10
SMILES:	CCCCCCO[C@H]1O[C@@H](COC(=O)C(F)(F)F)[C@H](OC(=O)C(F)(F)F)[C@@H](OC
Mol. weight [g/mol]:	648.35

Physical Properties

Property code	Value	Unit	Source
hfus	71.29	kJ/mol	Joback Method
logp	3.836		Crippen Method
mcpvol	344.540	ml/mol	McGowan Method
tb	598.27	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R190699>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
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
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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<https://www.chemeo.com/cid/117-108-2/Hexanol-beta-D-glucopyranoside-TFA.pdf>

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