(S)-2-Methylbutyl glucuronide, PFP

Inchi: InChI=1S/C20H17F15O10/c1-3-5(2)4-41-11-9(45-14(40)17(25,26)20(33,34)35)7(44-13(3

InchiKey: ZLYIYJQPJVWHOJ-ZAIAIYBWSA-N

Formula: C20H17F15O10

SMILES: CCC(C)COC1OC(C(=O)O)C(OC(=O)C(F)(F)C(F)(F)F)C(OC(=O)C(F)(F)C(F)(F)F)C1OC(

Mol. weight [g/mol]: 702.32

Physical Properties

Property code	Value	Unit	Source
gf	-3955.04	kJ/mol	Joback Method
hf	-4746.03	kJ/mol	Joback Method
hfus	65.08	kJ/mol	Joback Method
hvap	96.70	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.187		Crippen Method
mcvol	349.850	ml/mol	McGowan Method
pc	890.54	kPa	Joback Method
rinpol	1593.00		NIST Webbook
tb	1051.39	K	Joback Method
tc	1334.81	K	Joback Method
tf	689.98	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1259.21	J/mol×K	1051.39	Joback Method
cpg	1268.58	J/mol×K	1098.63	Joback Method
cpg	1276.01	J/mol×K	1145.86	Joback Method
cpg	1281.75	J/mol×K	1193.10	Joback Method
cpg	1286.02	J/mol×K	1240.34	Joback Method
cpg	1289.09	J/mol×K	1287.58	Joback Method
cpg	1291.18	J/mol×K	1334.81	Joback Method

Sources

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=R554786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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