

# (S)-2-Butyl glucuronide, PFP

<b>Inchi:</b>	InChI=1S/C19H15F15O10/c1-3-4(2)40-10-8(44-13(39)16(24,25)19(32,33)34)6(43-12(38)
<b>InchiKey:</b>	OGBPEWFEGQJNEI-VQMJRHPMSA-N
<b>Formula:</b>	C19H15F15O10
<b>SMILES:</b>	CCC(C)OC1OC(C(=O)O)C(OC(=O)C(F)(F)C(F)(F)F)C(OC(=O)C(F)(F)C(F)(F)F)C1OC(=
<b>Mol. weight [g/mol]:</b>	688.29

## Physical Properties

Property code	Value	Unit	Source
gf	-3963.46	kJ/mol	Joback Method
hf	-4725.39	kJ/mol	Joback Method
hfus	62.49	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	3.939		Crippen Method
mcvol	335.760	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinsol	1509.00		NIST Webbook
tb	1028.51	K	Joback Method
tc	1295.74	K	Joback Method
tf	678.71	K	Joback Method
vc	1.363	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1201.71	J/molxK	1028.51	Joback Method
cpg	1210.67	J/molxK	1073.05	Joback Method
cpg	1217.86	J/molxK	1117.59	Joback Method
cpg	1223.47	J/molxK	1162.12	Joback Method
cpg	1227.69	J/molxK	1206.66	Joback Method
cpg	1230.72	J/molxK	1251.20	Joback Method
cpg	1232.77	J/molxK	1295.74	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R554746&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R554746&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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