(R)-2-Butyl glucuronide, PFP

Inchi: InChI=1S/C19H15F15O10/c1-3-4(2)40-10-8(44-13(39)16(24,25)19(32,33)34)6(43-12(38)
InchiKey: OGBPEWFEGQJNEI-XDPSOMMASA-N
Formula: C19H15F15O10
SMILES: 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(=
Mol. weight [g/mol]: 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
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
tb	1028.51	K	Joback Method
tc	1295.74	K	Joback Method
tf	678.71	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554706&Units=SI
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

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