

Isopropyl glucuronide, PFP

Inchi:	InChI=1S/C18H13F15O10/c1-3(2)39-9-7(43-12(38)15(23,24)18(31,32)33)5(42-11(37)14
InchiKey:	WTCDUYAGQJUNJB-UHFFFAOYSA-N
Formula:	C18H13F15O10
SMILES:	CC(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(=O
Mol. weight [g/mol]:	674.27

Physical Properties

Property code	Value	Unit	Source
gf	-3971.88	kJ/mol	Joback Method
hf	-4704.75	kJ/mol	Joback Method
hfus	59.90	kJ/mol	Joback Method
hvap	92.25	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.549		Crippen Method
mvol	321.670	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
tb	1005.63	K	Joback Method
tc	1258.38	K	Joback Method
tf	667.44	K	Joback Method
vc	1.306	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1144.63	J/molxK	1005.63	Joback Method
cpg	1153.21	J/molxK	1047.76	Joback Method
cpg	1160.17	J/molxK	1089.88	Joback Method
cpg	1165.65	J/molxK	1132.01	Joback Method
cpg	1169.83	J/molxK	1174.13	Joback Method
cpg	1172.86	J/molxK	1216.26	Joback Method
cpg	1174.91	J/molxK	1258.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554588&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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