

Methyl glucuronide, PFP

Inchi: InChI=1S/C17H11F15O10/c1-37-7(33)5-3(40-9(34)12(18,19)15(24,25)26)4(41-10(35)13(36)14(38)39)/q1-10-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38-39-40-41/h1-17,20-23,26-29,32-35,38-41/t18,19,24,25,30,31,36,37,40,41/b1-17,20-23,26-29,32-35,38-41

InchiKey: VIHBWXQWOPROMY-UHFFFAOYSA-N

Formula: C17H11F15O10

SMILES: COC(=O)C1OC(OC)C(OC(=O)C(F)(F)C(F)(F)F)C(OC(=O)C(F)(F)C(F)(F)F)C1OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 660.24

Physical Properties

Property code	Value	Unit	Source
gf	-3946.04	kJ/mol	Joback Method
hf	-4658.82	kJ/mol	Joback Method
hfus	57.94	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	2.859		Crippen Method
mcvol	307.580	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	1357.00		NIST Webbook
rinpol	1357.00		NIST Webbook
tb	913.43	K	Joback Method
tc	1123.11	K	Joback Method
tf	632.58	K	Joback Method
vc	1.256	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.32	J/molxK	913.43	Joback Method
cpg	1079.14	J/molxK	948.38	Joback Method
cpg	1087.53	J/molxK	983.32	Joback Method
cpg	1094.56	J/molxK	1018.27	Joback Method
cpg	1100.32	J/molxK	1053.22	Joback Method
cpg	1104.86	J/molxK	1088.17	Joback Method
cpg	1108.27	J/molxK	1123.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R554622&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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