

Ethyl glucuronide, PFP

Inchi:	InChI=1S/C17H11F15O10/c1-2-38-8-6(42-11(37)14(22,23)17(30,31)32)4(41-10(36)13(20
InchiKey:	KMNFLKNCKJTGLN-UHFFFAOYSA-N
Formula:	C17H11F15O10
SMILES:	CCOC1OC(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)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	660.24

Physical Properties

Property code	Value	Unit	Source
gf	-3977.86	kJ/mol	Joback Method
hf	-4678.83	kJ/mol	Joback Method
hfus	60.84	kJ/mol	Joback Method
hvap	90.41	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.161		Crippen Method
mvol	307.580	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	1398.00		NIST Webbook
rinpol	1398.00		NIST Webbook
tb	983.19	K	Joback Method
tc	1225.78	K	Joback Method
tf	671.17	K	Joback Method
vc	1.256	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.55	J/molxK	983.19	Joback Method
cpg	1095.92	J/molxK	1023.62	Joback Method
cpg	1102.78	J/molxK	1064.05	Joback Method
cpg	1108.26	J/molxK	1104.49	Joback Method
cpg	1112.51	J/molxK	1144.92	Joback Method
cpg	1115.65	J/molxK	1185.35	Joback Method
cpg	1117.84	J/molxK	1225.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554464&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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