Propyl glucuronide, PFP

Inchi: InChI=1S/C18H13F15O10/c1-2-3-39-9-7(43-12(38)15(23,24)18(31,32)33)5(42-11(37)14(
InchiKey: UVGKCKBEUZWXED-UHFFFAOYSA-N
Formula: C18H13F15O10
SMILES: CCCOC1OC(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
Mol. weight [g/mol]: 674.27

Physical Properties

Property code	Value	Unit	Source
gf	-3969.44	kJ/mol	Joback Method
hf	-4699.47	kJ/mol	Joback Method
hfus	63.43	kJ/mol	Joback Method
hvap	92.64	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.551		Crippen Method
mcvol	321.670	ml/mol	McGowan Method
pc	997.02	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
tb	1006.07	K	Joback Method
tc	1262.08	K	Joback Method
tf	682.44	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1144.20	J/mol×K	1006.07	Joback Method
cpg	1152.96	J/mol×K	1048.74	Joback Method
cpg	1160.08	J/mol×K	1091.41	Joback Method
cpg	1165.70	J/mol×K	1134.08	Joback Method
cpg	1170.01	J/mol×K	1176.75	Joback Method
cpg	1173.18	J/mol×K	1219.41	Joback Method
cpg	1175.36	J/mol×K	1262.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554662&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