N-(3-Bromo-4-hydroxy-phenyl)-4-nitro-benzenesu O,N-di(pentafluoropropionyl)-

InChI: InChI=1S/C18H7BrF10N2O7S/c19-11-7-9(3-6-12(11)38-14(33)16(22,23)18(27,28)29)30(
InChIKey: PSQBNIGRERUAML-UHFFFAOYSA-N
Formula: C18H7BrF10N2O7S
SMILES: O=C(Oc1ccc(N(C(=O)C(F)(F)C(F)(F)F)S(=O)(=O)c2ccc([N+](=O)[O-])cc2)cc1Br)C(F)(F)C
Mol. weight [g/mol]: 665.21

Physical Properties

Property code	Value	Unit	Source
gf	-2310.86	kJ/mol	Joback Method
hf	-2699.93	kJ/mol	Joback Method
hfus	65.87	kJ/mol	Joback Method
hvap	108.45	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	5.380		Crippen Method
mcvol	316.660	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	2347.00		NIST Webbook
tb	1067.70	K	Joback Method
tc	1307.28	K	Joback Method
tf	795.13	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.27	J/mol×K	1067.70	Joback Method
cpg	953.78	J/mol×K	1107.63	Joback Method
cpg	958.89	J/mol×K	1147.56	Joback Method
cpg	963.77	J/mol×K	1187.49	Joback Method
cpg	968.62	J/mol×K	1227.42	Joback Method
cpg	973.60	J/mol×K	1267.35	Joback Method
cpg	978.91	J/mol×K	1307.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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