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

InChI: InChI=1S/C16H7BrF6N2O7S/c17-11-7-9(3-6-12(11)32-14(27)16(21,22)23)24(13(26)15(1

InChIKey: QLBMEHHSFJQRMI-UHFFFAOYSA-N

Formula: C16H7BrF6N2O7S

SMILES: O=C(Oc1ccc(N(C(=O)C(F)(F)F)S(=O)(=O)c2ccc([N+](=O)[O-])cc2)cc1Br)C(F)(F)F

Mol. weight [g/mol]: 565.20

Physical Properties

Property code	Value	Unit	Source
gf	-1554.14	kJ/mol	Joback Method
hf	-1856.71	kJ/mol	Joback Method
hfus	63.19	kJ/mol	Joback Method
hvap	109.86	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	4.109		Crippen Method
mcvol	281.400	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	1031.32	K	Joback Method
tc	1269.48	K	Joback Method
tf	765.39	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.56	J/mol×K	1031.32	Joback Method
cpg	812.39	J/mol×K	1071.01	Joback Method
cpg	816.37	J/mol×K	1110.71	Joback Method
cpg	819.59	J/mol×K	1150.40	Joback Method
cpg	822.17	J/mol×K	1190.09	Joback Method
cpg	824.22	J/mol×K	1229.78	Joback Method
cpg	825.84	J/mol×K	1269.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374411&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