2,4-Diaminophenol, N,N',O-tris-(rifluoroacetyl)-

Other names: 2,4-Bis((trifluoroacetyl)amino)phenyl trifluoroacetate
Inchi: InChI=1S/C12H5F9N2O4/c13-10(14,15)7(24)22-4-1-2-6(27-9(26)12(19,20)21)5(3-4)23-8
InchiKey: ISMOVDOGCJJMNE-UHFFFAOYSA-N
Formula: C12H5F9N2O4
SMILES: O=C(Nc1ccc(OC(=O)C(F)(F)F)c(NC(=O)C(F)(F)F)c1)C(F)(F)F
Mol. weight [g/mol]: 412.16

Physical Properties

Property code	Value	Unit	Source
gf	-1914.44	kJ/mol	Joback Method
hf	-2231.68	kJ/mol	Joback Method
hfus	41.76	kJ/mol	Joback Method
hvap	70.18	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.156		Crippen Method
mcvol	202.650	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1508.00		NIST Webbook
tb	778.71	K	Joback Method
tc	966.45	K	Joback Method
tf	566.37	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.32	J/mol×K	778.71	Joback Method
cpg	607.08	J/mol×K	810.00	Joback Method
cpg	614.14	J/mol×K	841.29	Joback Method
cpg	620.56	J/mol×K	872.58	Joback Method
cpg	626.38	J/mol×K	903.87	Joback Method
cpg	631.67	J/mol×K	935.16	Joback Method
cpg	636.49	J/mol×K	966.45	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=U373247&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