5-Amino-2-methoxyphenol, N,N,O-tris(trifluoroacetyl)-

Inchi: InChI=1S/C13H6F9NO5/c1-27-6-3-2-5(4-7(6)28-10(26)13(20,21)22)23(8(24)11(14,15)16

InchiKey: JELDXANQGKOGEG-UHFFFAOYSA-N

Formula: C13H6F9NO5

SMILES: COc1ccc(N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)cc1OC(=O)C(F)(F)F

Mol. weight [g/mol]: 427.18

Physical Properties

Property code	Value	Unit	Source
gf	-2079.02	kJ/mol	Joback Method
hf	-2423.95	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	63.99	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.147		Crippen Method
mcvol	212.630	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	1273.00		NIST Webbook
rinpol	1273.00		NIST Webbook
tb	736.11	K	Joback Method
tc	916.41	K	Joback Method
tf	527.02	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.03	J/mol×K	736.11	Joback Method
cpg	627.12	J/mol×K	766.16	Joback Method
cpg	635.45	J/mol×K	796.21	Joback Method
cpg	643.08	J/mol×K	826.26	Joback Method
cpg	650.03	J/mol×K	856.31	Joback Method
cpg	656.37	J/mol×K	886.36	Joback Method
cpg	662.13	J/mol×K	916.41	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=U374875&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