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

Inchi: InChI=1S/C16H6F15NO5/c1-36-6-3-2-5(4-7(6)37-10(35)13(21,22)16(29,30)31)32(8(33)1

InchiKey: FBRQMXRLZNMRDL-UHFFFAOYSA-N

Formula: C16H6F15NO5

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

Mol. weight [g/mol]: 577.20

Physical Properties

Property code	Value	Unit	Source
gf	-3214.10	kJ/mol	Joback Method
hf	-3688.78	kJ/mol	Joback Method
hfus	42.37	kJ/mol	Joback Method
hvap	61.88	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.053		Crippen Method
mcvol	265.520	ml/mol	McGowan Method
pc	1221.70	kPa	Joback Method
rinpol	1262.00		NIST Webbook
rinpol	1262.00		NIST Webbook
tb	790.68	K	Joback Method
tc	969.06	K	Joback Method
tf	571.63	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.22	J/mol×K	790.68	Joback Method
cpg	837.97	J/mol×K	820.41	Joback Method
cpg	845.92	J/mol×K	850.14	Joback Method
cpg	853.17	J/mol×K	879.87	Joback Method
cpg	859.81	J/mol×K	909.60	Joback Method
cpg	865.92	J/mol×K	939.33	Joback Method
cpg	871.59	J/mol×K	969.06	Joback Method

Sources

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=U374470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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