5-Amino-2-methoxyphenol, N-pentafluoropropionyl-

Inchi: InChI=1S/C10H8F5NO3/c1-19-7-3-2-5(4-6(7)17)16-8(18)9(11,12)10(13,14)15/h2-4,17H,1

InchiKey: QELZYGIRPCHCOA-UHFFFAOYSA-N

Formula: C10H8F5NO3

SMILES: COc1ccc(NC(=O)C(F)(F)C(F)(F)F)cc1O

Mol. weight [g/mol]: 285.17

Physical Properties

Property code	Value	Unit	Source
gf	-1131.42	kJ/mol	Joback Method
hf	-1391.36	kJ/mol	Joback Method
hfus	29.55	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.537		Crippen Method
mcvol	160.140	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	656.83	K	Joback Method
tc	856.63	K	Joback Method
tf	485.73	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.54	J/mol×K	656.83	Joback Method
cpg	453.32	J/mol×K	690.13	Joback Method
cpg	462.35	J/mol×K	723.43	Joback Method
cpg	470.70	J/mol×K	756.73	Joback Method
cpg	478.46	J/mol×K	790.03	Joback Method
cpg	485.71	J/mol×K	823.33	Joback Method
cpg	492.52	J/mol×K	856.63	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=U374471&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