5-Amino-2-methoxyphenol, N-trifluoroacetyl-

Inchi: InChI=1S/C9H8F3NO3/c1-16-7-3-2-5(4-6(7)14)13-8(15)9(10,11)12/h2-4,14H,1H3,(H,13,1
InchiKey: PVJGTMBCIOHIFG-UHFFFAOYSA-N
Formula: C9H8F3NO3
SMILES: COc1ccc(NC(=O)C(F)(F)F)cc1O
Mol. weight [g/mol]: 235.16

Physical Properties

Property code	Value	Unit	Source
gf	-753.06	kJ/mol	Joback Method
hf	-969.75	kJ/mol	Joback Method
hfus	28.21	kJ/mol	Joback Method
hvap	63.42	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.902		Crippen Method
mcvol	142.510	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	1681.00		NIST Webbook
tb	638.64	K	Joback Method
tc	848.13	K	Joback Method
tf	470.86	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.85	J/mol×K	638.64	Joback Method
cpg	385.61	J/mol×K	673.55	Joback Method
cpg	394.65	J/mol×K	708.47	Joback Method
cpg	403.05	J/mol×K	743.38	Joback Method
cpg	410.88	J/mol×K	778.30	Joback Method
cpg	418.20	J/mol×K	813.21	Joback Method
cpg	425.08	J/mol×K	848.13	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=U374880&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