5-Amino-2-methoxyphenol, N-heptafluorobutyryl-

Inchi: InChI=1S/C11H8F7NO3/c1-22-7-3-2-5(4-6(7)20)19-8(21)9(12,13)10(14,15)11(16,17)18/h

InchiKey: YWQNZDCGJOMTNU-UHFFFAOYSA-N

Formula: C11H8F7NO3

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

Mol. weight [g/mol]: 335.17

Physical Properties

Property code	Value	Unit	Source
gf	-1509.78	kJ/mol	Joback Method
hf	-1812.97	kJ/mol	Joback Method
hfus	30.89	kJ/mol	Joback Method
hvap	62.02	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.172		Crippen Method
mcvol	177.770	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1565.00		NIST Webbook
rinpol	1565.00		NIST Webbook
tb	675.02	K	Joback Method
tc	866.68	K	Joback Method
tf	500.60	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.96	J/mol×K	675.02	Joback Method
cpg	521.68	J/mol×K	706.96	Joback Method
cpg	530.62	J/mol×K	738.91	Joback Method
cpg	538.87	J/mol×K	770.85	Joback Method
cpg	546.53	J/mol×K	802.79	Joback Method
cpg	553.69	J/mol×K	834.73	Joback Method
cpg	560.42	J/mol×K	866.68	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U374472&Units=SI

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