5-Amino-2-methoxyphenol, O,N-bis(heptafluorobutyryl)-

Inchi: InChI=1S/C15H7F14NO4/c1-33-6-3-2-5(30-8(31)10(16,17)12(20,21)14(24,25)26)4-7(6)3
InchiKey: WWEMBNJLHOZZRA-UHFFFAOYSA-N
Formula: C15H7F14NO4
SMILES: COc1ccc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 531.20

Physical Properties

Property code	Value	Unit	Source
gf	-2920.18	kJ/mol	Joback Method
hf	-3373.51	kJ/mol	Joback Method
hfus	37.18	kJ/mol	Joback Method
hvap	58.12	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.205		Crippen Method
mcvol	248.090	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	1524.00		NIST Webbook
rinpol	1524.00		NIST Webbook
tb	752.39	K	Joback Method
tc	926.11	K	Joback Method
tf	530.03	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.06	J/mol×K	752.39	Joback Method
cpg	778.41	J/mol×K	781.34	Joback Method
cpg	786.94	J/mol×K	810.30	Joback Method
cpg	794.74	J/mol×K	839.25	Joback Method
cpg	801.89	J/mol×K	868.20	Joback Method
cpg	808.46	J/mol×K	897.15	Joback Method
cpg	814.53	J/mol×K	926.11	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=U374876&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