4-Aminobenzoic acid, N,O-bis(pentafluoropropionyl)-

Inchi: InChI=1S/C13H5F10NO4/c14-10(15,12(18,19)20)8(26)24-6-3-1-5(2-4-6)7(25)28-9(27)11

InchiKey: ZHCVZWKXNNLIDU-UHFFFAOYSA-N

Formula: C13H5F10NO4

SMILES: O=C(OC(=O)C(F)(F)C(F)(F)F)c1ccc(NC(=O)C(F)(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 429.17

Physical Properties

Property code	Value	Unit	Source
gf	-2177.75	kJ/mol	Joback Method
hf	-2499.18	kJ/mol	Joback Method
hfus	35.31	kJ/mol	Joback Method
hvap	63.20	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.704		Crippen Method
mcvol	208.530	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
tb	742.48	K	Joback Method
tc	926.16	K	Joback Method
tf	515.47	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.87	J/mol×K	742.48	Joback Method
cpg	624.32	J/mol×K	773.09	Joback Method
cpg	631.99	J/mol×K	803.71	Joback Method
cpg	638.95	J/mol×K	834.32	Joback Method
cpg	645.28	J/mol×K	864.93	Joback Method
cpg	651.05	J/mol×K	895.55	Joback Method
cpg	656.33	J/mol×K	926.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375076&Units=SI
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

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