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

Inchi: InChI=1S/C11H5F6NO4/c12-10(13,14)8(20)18-6-3-1-5(2-4-6)7(19)22-9(21)11(15,16)17/h
InchiKey: JHXIHVYKFWOXHJ-UHFFFAOYSA-N
Formula: C11H5F6NO4
SMILES: O=C(OC(=O)C(F)(F)F)c1ccc(NC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 329.15

Physical Properties

Property code	Value	Unit	Source
gf	-1421.03	kJ/mol	Joback Method
hf	-1655.96	kJ/mol	Joback Method
hfus	32.63	kJ/mol	Joback Method
hvap	64.61	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.433		Crippen Method
mcvol	173.270	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	1488.00		NIST Webbook
tb	706.10	K	Joback Method
tc	900.50	K	Joback Method
tf	485.73	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.35	J/mol×K	706.10	Joback Method
cpg	486.12	J/mol×K	738.50	Joback Method
cpg	494.12	J/mol×K	770.90	Joback Method
cpg	501.41	J/mol×K	803.30	Joback Method
cpg	508.04	J/mol×K	835.70	Joback Method
cpg	514.04	J/mol×K	868.10	Joback Method
cpg	519.48	J/mol×K	900.50	Joback Method

Sources

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=U375077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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