4-(Nonafluoro-tert-butyl) aniline

Inchi: InChI=1S/C10H6F9N/c11-8(12,13)7(9(14,15)16,10(17,18)19)5-1-3-6(20)4-2-5/h1-4H,20H
InchiKey: ODNSTTKMCKKBOI-UHFFFAOYSA-N
Formula: C10H6F9N
SMILES: Nc1ccc(C(C(F)(F)F)(C(F)(F)F)C(F)(F)F)cc1
Mol. weight [g/mol]: 311.15
CAS: 41125-50-2

Physical Properties

Property code	Value	Unit	Source
gf	-1539.38	kJ/mol	Joback Method
hf	-1790.87	kJ/mol	Joback Method
hfus	18.57	kJ/mol	Joback Method
hvap	38.90	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.194		Crippen Method
mcvol	153.910	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
tb	512.90	K	Joback Method
tc	689.52	K	Joback Method
tf	339.65	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.41	J/mol×K	512.90	Joback Method
cpg	416.10	J/mol×K	542.34	Joback Method
cpg	427.71	J/mol×K	571.77	Joback Method
cpg	438.32	J/mol×K	601.21	Joback Method
cpg	448.01	J/mol×K	630.65	Joback Method
cpg	456.83	J/mol×K	660.08	Joback Method
cpg	464.85	J/mol×K	689.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41125502&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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