

Aniline, o-[5-chloro-(2,2,3,3,4,4-hexafluoro-cyclopenten-1-

Inchi:	InChI=1S/C11H6ClF6NS/c12-7-8(20-6-4-2-1-3-5(6)19)10(15,16)11(17,18)9(7,13)14/h1-4
InchiKey:	PEGJNVBCOCWFKU-UHFFFAOYSA-N
Formula:	C11H6ClF6NS
SMILES:	Nc1ccccc1SC1=C(Cl)C(F)(F)C(F)(F)C1(F)F
Mol. weight [g/mol]:	333.68
CAS:	116277-71-5

Physical Properties

Property code	Value	Unit	Source
gf	-921.34	kJ/mol	Joback Method
hf	-1061.69	kJ/mol	Joback Method
hfus	27.53	kJ/mol	Joback Method
hvap	57.76	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.731		Crippen Method
mcvol	176.120	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	672.88	K	Joback Method
tc	902.31	K	Joback Method
tf	503.71	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.98	J/molxK	672.88	Joback Method
cpg	458.80	J/molxK	711.12	Joback Method
cpg	469.50	J/molxK	749.36	Joback Method
cpg	480.41	J/molxK	787.59	Joback Method
cpg	491.85	J/molxK	825.83	Joback Method
cpg	504.14	J/molxK	864.07	Joback Method
cpg	517.63	J/molxK	902.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116277715&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
mccvol:	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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