3-(Pentafluoropropionylthio)benzoyl chloride

Inchi: InChI=1S/C10H4ClF5O2S/c11-7(17)5-2-1-3-6(4-5)19-8(18)9(12,13)10(14,15)16/h1-4H
InchiKey: KAUIESJINPEJGR-UHFFFAOYSA-N
Formula: C10H4ClF5O2S
SMILES: O=C(Cl)c1cccc(SC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 318.65

Physical Properties

Property code	Value	Unit	Source
gf	-1068.92	kJ/mol	Joback Method
hf	-1221.75	kJ/mol	Joback Method
hfus	27.41	kJ/mol	Joback Method
hvap	58.81	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.882		Crippen Method
mcvol	168.580	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
tb	663.70	K	Joback Method
tc	882.12	K	Joback Method
tf	413.37	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.42	J/mol×K	663.70	Joback Method
cpg	418.44	J/mol×K	700.10	Joback Method
cpg	426.56	J/mol×K	736.51	Joback Method
cpg	433.85	J/mol×K	772.91	Joback Method
cpg	440.38	J/mol×K	809.31	Joback Method
cpg	446.21	J/mol×K	845.72	Joback Method
cpg	451.42	J/mol×K	882.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375149&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