N-(3-Chlorophenyl)-N-(trifluoroacetyl)-2,2,2-trifluo

Inchi: InChI=1S/C10H4ClF6NO2/c11-5-2-1-3-6(4-5)18(7(19)9(12,13)14)8(20)10(15,16)17/h1-4
InchiKey: YOMBILLCPMCEND-UHFFFAOYSA-N
Formula: C10H4ClF6NO2
SMILES: O=C(N(C(=O)C(F)(F)F)c1cccc(Cl)c1)C(F)(F)F
Mol. weight [g/mol]: 319.59

Physical Properties

Property code	Value	Unit	Source
gf	-1186.07	kJ/mol	Joback Method
hf	-1392.20	kJ/mol	Joback Method
hfus	29.38	kJ/mol	Joback Method
hvap	53.22	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.324		Crippen Method
mcvol	163.980	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	1135.00		NIST Webbook
rinpol	1135.00		NIST Webbook
tb	606.63	K	Joback Method
tc	797.88	K	Joback Method
tf	412.03	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.29	J/mol×K	606.63	Joback Method
cpg	418.02	J/mol×K	638.50	Joback Method
cpg	426.90	J/mol×K	670.38	Joback Method
cpg	434.99	J/mol×K	702.25	Joback Method
cpg	442.34	J/mol×K	734.13	Joback Method
cpg	449.03	J/mol×K	766.00	Joback Method
cpg	455.10	J/mol×K	797.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373269&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