Benzene, (1,2-dichloro-1,2,2-trifluoroethyl)-3,5-bis-(trifluoro

Inchi: InChI=1S/C10H3Cl2F9/c11-7(13,10(12,20)21)4-1-5(8(14,15)16)3-6(2-4)9(17,18)19/h1-3H

InchiKey: DZIGRGRUXUJJAW-UHFFFAOYSA-N

Formula: C10H3Cl2F9

SMILES: FC(F)(F)c1cc(C(F)(F)F)cc(C(F)(Cl)C(F)(F)Cl)c1

Mol. weight [g/mol]: 365.02

Physical Properties

Property code	Value	Unit	Source
gf	-1639.32	kJ/mol	Joback Method
hf	-1867.61	kJ/mol	Joback Method
hfus	21.38	kJ/mol	Joback Method
hvap	37.69	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.917		Crippen Method
mcvol	168.410	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	895.00		NIST Webbook
tb	520.21	K	Joback Method
tc	697.93	K	Joback Method
tf	328.75	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.50	J/mol×K	520.21	Joback Method
cpg	411.55	J/mol×K	549.83	Joback Method
cpg	421.60	J/mol×K	579.45	Joback Method
cpg	430.72	J/mol×K	609.07	Joback Method
cpg	438.98	J/mol×K	638.69	Joback Method
cpg	446.45	J/mol×K	668.31	Joback Method
cpg	453.20	J/mol×K	697.93	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=R504177&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