Benzene, 1-nitro-4-(2,2,2-trichloroethyl)

Inchi: InChI=1S/C8H6Cl3NO2/c9-8(10,11)5-6-1-3-7(4-2-6)12(13)14/h1-4H,5H2
InchiKey: GRXKQNJAZNVHAH-UHFFFAOYSA-N
Formula: C8H6Cl3NO2
SMILES: O=[N+]([O-])c1ccc(CC(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]: 254.50

Physical Properties

Property code	Value	Unit	Source
gf	121.86	kJ/mol	Joback Method
hf	-50.12	kJ/mol	Joback Method
hfus	26.67	kJ/mol	Joback Method
hvap	64.79	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.508		Crippen Method
mcvol	153.960	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
rinpol	1758.00		NIST Webbook
tb	675.00	K	Joback Method
tc	945.09	K	Joback Method
tf	454.65	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.13	J/mol×K	675.00	Joback Method
cpg	342.56	J/mol×K	720.02	Joback Method
cpg	350.98	J/mol×K	765.03	Joback Method
cpg	358.51	J/mol×K	810.05	Joback Method
cpg	365.26	J/mol×K	855.06	Joback Method
cpg	371.34	J/mol×K	900.08	Joback Method
cpg	376.86	J/mol×K	945.09	Joback Method

Sources

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=R515147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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