3,5-Dinitrobenzyl alcohol, chlorodifluoroacetate

Inchi: InChI=1S/C9H5ClF2N2O6/c10-9(11,12)8(15)20-4-5-1-6(13(16)17)3-7(2-5)14(18)19/h1-3
InchiKey: CUCJMXIHFQZJMF-UHFFFAOYSA-N
Formula: C9H5ClF2N2O6
SMILES: O=C(OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1)C(F)(F)Cl
Mol. weight [g/mol]: 310.60

Physical Properties

Property code	Value	Unit	Source
gf	-443.48	kJ/mol	Joback Method
hf	-698.53	kJ/mol	Joback Method
hfus	40.78	kJ/mol	Joback Method
hvap	83.02	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	2.378		Crippen Method
mcvol	171.970	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	854.67	K	Joback Method
tc	1108.81	K	Joback Method
tf	635.55	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.90	J/mol×K	854.67	Joback Method
cpg	469.03	J/mol×K	897.03	Joback Method
cpg	475.30	J/mol×K	939.38	Joback Method
cpg	480.77	J/mol×K	981.74	Joback Method
cpg	485.51	J/mol×K	1024.10	Joback Method
cpg	489.58	J/mol×K	1066.46	Joback Method
cpg	493.04	J/mol×K	1108.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376143&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
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