2,2-Dichloroethyl 3,5-dinitrobenzoate

Other names: Benzoic acid, 3,5-dinitro, 2,2-dichloroethyl ester
Inchi: InChI=1S/C9H6Cl2N2O6/c10-8(11)4-19-9(14)5-1-6(12(15)16)3-7(2-5)13(17)18/h1-3,8H,4
InchiKey: HLDOIZVVCCPUCS-UHFFFAOYSA-N
Formula: C9H6Cl2N2O6
SMILES: O=C(OCC(Cl)Cl)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 309.06

Physical Properties

Property code	Value	Unit	Source
gf	-71.07	kJ/mol	Joback Method
hf	-318.58	kJ/mol	Joback Method
hfus	42.71	kJ/mol	Joback Method
hvap	89.95	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	2.464		Crippen Method
mcvol	180.670	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	2099.00		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	896.35	K	Joback Method
tc	1164.19	K	Joback Method
tf	646.87	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.59	J/mol×K	896.35	Joback Method
cpg	468.50	J/mol×K	940.99	Joback Method
cpg	474.41	J/mol×K	985.63	Joback Method
cpg	479.35	J/mol×K	1030.27	Joback Method

cpg	483.36	J/mol×K	1074.91	Joback Method
cpg	486.47	J/mol×K	1119.55	Joback Method
cpg	488.73	J/mol×K	1164.19	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=U373864&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