

2-Chloroethyl 3,5-dinitrobenzoate

Other names:	Benzoic acid, 3,5-dinitro, 2-chloroethyl ester
Inchi:	InChI=1S/C9H7ClN2O6/c10-1-2-18-9(13)6-3-7(11(14)15)5-8(4-6)12(16)17/h3-5H,1-2H2
InchiKey:	NMYQUFDBMCNAHO-UHFFFAOYSA-N
Formula:	C9H7ClN2O6
SMILES:	O=C(OCCCl)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	274.62

Physical Properties

Property code	Value	Unit	Source
gf	-56.70	kJ/mol	Joback Method
hf	-297.56	kJ/mol	Joback Method
hfus	42.03	kJ/mol	Joback Method
hvap	85.95	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	1.899		Crippen Method
mcvol	168.430	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	2015.00		NIST Webbook
rinpol	2014.00		NIST Webbook
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook
tb	859.36	K	Joback Method
tc	1121.29	K	Joback Method
tf	631.95	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.00	J/molxK	859.36	Joback Method
cpg	453.00	J/molxK	903.01	Joback Method
cpg	460.01	J/molxK	946.67	Joback Method
cpg	466.07	J/molxK	990.32	Joback Method
cpg	471.21	J/molxK	1033.98	Joback Method

cpg	475.45	J/mol×K	1077.63	Joback Method
cpg	478.82	J/mol×K	1121.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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