Benzoic acid, 4-nitro, 2,2,2-trichloroethyl ester

Other names: Ethanol, 2,2,2-trichloro, 4-nitrobenzoate
Inchi: InChI=1S/C9H6Cl3NO4/c10-9(11,12)5-17-8(14)6-1-3-7(4-2-6)13(15)16/h1-4H,5H2
InchiKey: ZXPRNGMQBLDZQB-UHFFFAOYSA-N
Formula: C9H6Cl3NO4
SMILES: O=C(OCC(Cl)(Cl)Cl)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 298.51

Physical Properties

Property code	Value	Unit	Source
gf	-103.64	kJ/mol	Joback Method
hf	-315.56	kJ/mol	Joback Method
hfus	32.04	kJ/mol	Joback Method
hvap	76.17	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.122		Crippen Method
mcvol	175.490	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	1867.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1891.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1891.00		NIST Webbook
ripol	2904.00		NIST Webbook
ripol	2847.00		NIST Webbook
ripol	2873.00		NIST Webbook
ripol	2867.00		NIST Webbook
ripol	2847.00		NIST Webbook
ripol	2867.00		NIST Webbook
tb	774.17	K	Joback Method
tc	1037.32	K	Joback Method
tf	538.08	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.50	J/mol×K	774.17	Joback Method
cpg	416.78	J/mol×K	818.03	Joback Method
cpg	424.13	J/mol×K	861.89	Joback Method
cpg	430.64	J/mol×K	905.75	Joback Method
cpg	436.37	J/mol×K	949.60	Joback Method
cpg	441.41	J/mol×K	993.46	Joback Method
cpg	445.84	J/mol×K	1037.32	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R34810&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume