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

Other names: Ethanol, 2,2-dichloro, 4-nitrobenzoate
Inchi: InChI=1S/C9H7Cl2NO4/c10-8(11)5-16-9(13)6-1-3-7(4-2-6)12(14)15/h1-4,8H,5H2
InchiKey: JIPLOCBYOXAWRX-UHFFFAOYSA-N
Formula: C9H7Cl2NO4
SMILES: O=C(OCC(Cl)Cl)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 264.06

Physical Properties

Property code	Value	Unit	Source
gf	-96.99	kJ/mol	Joback Method
hf	-296.35	kJ/mol	Joback Method
hfus	31.74	kJ/mol	Joback Method
hvap	72.70	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.555		Crippen Method
mcvol	163.250	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1821.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1809.00		NIST Webbook
ripol	2913.00		NIST Webbook
ripol	2913.00		NIST Webbook
ripol	2940.00		NIST Webbook
ripol	2940.00		NIST Webbook
ripol	2965.00		NIST Webbook
ripol	2938.00		NIST Webbook
tb	739.53	K	Joback Method
tc	991.47	K	Joback Method
tf	490.74	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.90	J/mol×K	739.53	Joback Method
cpg	397.42	J/mol×K	781.52	Joback Method
cpg	406.02	J/mol×K	823.51	Joback Method
cpg	413.74	J/mol×K	865.50	Joback Method
cpg	420.62	J/mol×K	907.49	Joback Method
cpg	426.67	J/mol×K	949.48	Joback Method
cpg	431.94	J/mol×K	991.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R34824&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

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