

Benzoic acid, 4-nitro, 2-chloroethyl ester

Other names:	Ethanol, 2-chloro, 4-nitrobenzoate
Inchi:	InChI=1S/C9H8ClNO4/c10-5-6-15-9(12)7-1-3-8(4-2-7)11(13)14/h1-4H,5-6H2
InchiKey:	BUIVPELJVUWILR-UHFFFAOYSA-N
Formula:	C9H8ClNO4
SMILES:	O=C(OCCCl)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	229.62
CAS:	949-03-1

Physical Properties

Property code	Value	Unit	Source
gf	-82.62	kJ/mol	Joback Method
hf	-275.33	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	68.70	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	1.990		Crippen Method
mcvol	151.010	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1732.00		NIST Webbook
ripol	2821.00		NIST Webbook
ripol	2860.00		NIST Webbook
ripol	2831.00		NIST Webbook
ripol	2808.00		NIST Webbook
tb	702.54	K	Joback Method
tc	947.37	K	Joback Method
tf	475.82	K	Joback Method
vc	0.587	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	367.31	J/mol×K	702.54	Joback Method
cpg	377.71	J/mol×K	743.35	Joback Method
cpg	387.23	J/mol×K	784.15	Joback Method
cpg	395.91	J/mol×K	824.96	Joback Method
cpg	403.76	J/mol×K	865.76	Joback Method
cpg	410.81	J/mol×K	906.57	Joback Method
cpg	417.10	J/mol×K	947.37	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=C949031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
ripol:	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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