

Ethanol, 2,2,2-trichloro-, benzoate

Other names:	Trichloroethyl benzoate Benzoic acid, 2,2,2-trichloroethyl ester 2,2,2-Trichloroethyl benzoate
Inchi:	InChI=1S/C9H7Cl3O2/c10-9(11,12)6-14-8(13)7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	WGXLSZQUOYSATB-UHFFFAOYSA-N
Formula:	C9H7Cl3O2
SMILES:	O=C(OCC(Cl)(Cl)Cl)c1ccccc1
Mol. weight [g/mol]:	253.51
CAS:	37934-99-9

Physical Properties

Property code	Value	Unit	Source
gf	-129.56	kJ/mol	Joback Method
hf	-293.33	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	58.92	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.214		Crippen Method
mcvol	158.070	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1552.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1530.00		NIST Webbook
ripol	2159.00		NIST Webbook
ripol	2199.00		NIST Webbook
ripol	2199.00		NIST Webbook

ripol	2239.00		NIST Webbook
ripol	2205.00		NIST Webbook
ripol	2159.00		NIST Webbook
tb	617.35	K	Joback Method
tc	860.55	K	Joback Method
tf	381.95	K	Joback Method
vc	0.592	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.31	J/molxK	617.35	Joback Method
cpg	341.86	J/molxK	657.88	Joback Method
cpg	351.45	J/molxK	698.42	Joback Method
cpg	360.15	J/molxK	738.95	Joback Method
cpg	368.01	J/molxK	779.48	Joback Method
cpg	375.11	J/molxK	820.01	Joback Method
cpg	381.49	J/molxK	860.55	Joback Method
dvisc	0.0018809	Paxs	381.95	Joback Method
dvisc	0.0010697	Paxs	421.18	Joback Method
dvisc	0.0006698	Paxs	460.42	Joback Method
dvisc	0.0004514	Paxs	499.65	Joback Method
dvisc	0.0003222	Paxs	538.88	Joback Method
dvisc	0.0002407	Paxs	578.12	Joback Method
dvisc	0.0001867	Paxs	617.35	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C37934999&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
dvisc:	Dynamic viscosity
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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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