

Benzoic acid, 3-methyl-, 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C10H9Cl3O2/c1-7-3-2-4-8(5-7)9(14)15-6-10(11,12)13/h2-5H,6H2,1H3
InchiKey:	MDVZGTHFISDBQE-UHFFFAOYSA-N
Formula:	C10H9Cl3O2
SMILES:	Cc1cccc(C(=O)OCC(Cl)(Cl)Cl)c1
Mol. weight [g/mol]:	267.54

Physical Properties

Property code	Value	Unit	Source
gf	-130.77	kJ/mol	Joback Method
hf	-325.44	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	61.81	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.522		Crippen Method
mcvol	172.160	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinqol	1703.00		NIST Webbook
tb	645.21	K	Joback Method
tc	884.19	K	Joback Method
tf	405.74	K	Joback Method
vc	0.647	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.75	J/molxK	645.21	Joback Method
cpg	423.59	J/molxK	844.36	Joback Method
cpg	415.86	J/molxK	804.53	Joback Method
cpg	407.37	J/molxK	764.70	Joback Method
cpg	398.05	J/molxK	724.87	Joback Method
cpg	387.87	J/molxK	685.04	Joback Method
cpg	430.61	J/molxK	884.19	Joback Method
dvisc	0.0001612	Paxs	645.21	Joback Method
dvisc	0.0002051	Paxs	605.30	Joback Method

dvisc	0.0002700	Paxs	565.39	Joback Method
dvisc	0.0003706	Paxs	525.48	Joback Method
dvisc	0.0005359	Paxs	485.56	Joback Method
dvisc	0.0008277	Paxs	445.65	Joback Method
dvisc	0.0013925	Paxs	405.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355709&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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