

1,3,5-Benzenetricarbonyl trichloride

Other names:	Trimesoyl chloride 1,3,5-Benzenetricarboxylic acid chloride 1,3,5-Benzenetricarbonyl chloride Benzenetricarbonyl chloride Trimesic acid trichloride 1,3,5-Benzenetricarboxylic chloride benzene-1,3,5-tricarbonyl trichloride
Inchi:	InChI=1S/C9H3Cl3O3/c10-7(13)4-1-5(8(11)14)3-6(2-4)9(12)15/h1-3H
InchiKey:	UWCPYKQBIPYOLX-UHFFFAOYSA-N
Formula:	C9H3Cl3O3
SMILES:	O=C(Cl)c1cc(C(=O)Cl)cc(C(=O)Cl)c1
Mol. weight [g/mol]:	265.48
CAS:	4422-95-1

Physical Properties

Property code	Value	Unit	Source
gf	-304.50	kJ/mol	Joback Method
hf	-400.46	kJ/mol	Joback Method
hfus	29.72	kJ/mol	Joback Method
hvap	72.62	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	2.824		Crippen Method
mcvol	155.340	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
tb	715.86	K	Joback Method
tc	961.95	K	Joback Method
tf	482.20	K	Joback Method
vc	0.597	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.36	J/mol×K	715.86	Joback Method
cpg	322.40	J/mol×K	756.87	Joback Method

cpg	328.75	J/molxK	797.89	Joback Method
cpg	334.43	J/molxK	838.90	Joback Method
cpg	339.48	J/molxK	879.92	Joback Method
cpg	343.93	J/molxK	920.93	Joback Method
cpg	347.80	J/molxK	961.95	Joback Method
dvisc	0.0013241	Paxs	482.20	Joback Method
dvisc	0.0009212	Paxs	521.14	Joback Method
dvisc	0.0006741	Paxs	560.09	Joback Method
dvisc	0.0005137	Paxs	599.03	Joback Method
dvisc	0.0004046	Paxs	637.97	Joback Method
dvisc	0.0003276	Paxs	676.92	Joback Method
dvisc	0.0002714	Paxs	715.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	459.00 ± 1.00	K	1.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4422951&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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