

2,2,3-Trichloropropionic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C9H3Cl7O2/c10-2-9(15,16)8(17)18-7-4(12)1-3(11)5(13)6(7)14/h1H,2H2
InchiKey:	YWASYKJXJBUOOA-UHFFFAOYSA-N
Formula:	C9H3Cl7O2
SMILES:	O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)C(Cl)(Cl)CCl
Mol. weight [g/mol]:	391.29

Physical Properties

Property code	Value	Unit	Source
gf	-215.80	kJ/mol	Joback Method
hf	-402.17	kJ/mol	Joback Method
hfus	36.30	kJ/mol	Joback Method
hvap	79.11	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.618		Crippen Method
mcvol	207.030	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
tb	786.99	K	Joback Method
tc	1042.57	K	Joback Method
tf	551.71	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.79	J/molxK	786.99	Joback Method
cpg	402.64	J/molxK	829.59	Joback Method
cpg	407.83	J/molxK	872.18	Joback Method
cpg	412.39	J/molxK	914.78	Joback Method
cpg	416.38	J/molxK	957.38	Joback Method
cpg	419.84	J/molxK	999.97	Joback Method
cpg	422.80	J/molxK	1042.57	Joback Method
dvisc	0.0004829	Paxs	551.71	Joback Method
dvisc	0.0003451	Paxs	590.92	Joback Method
dvisc	0.0002571	Paxs	630.14	Joback Method

dvisc	0.0001983	Paxs	669.35	Joback Method
dvisc	0.0001574	Paxs	708.56	Joback Method
dvisc	0.0001280	Paxs	747.78	Joback Method
dvisc	0.0001062	Paxs	786.99	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003927&Units=SI

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
hvac:	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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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