

2,4,5-Trichlorophenyl trichloroacetate

Inchi:	InChI=1S/C8H2Cl6O2/c9-3-1-5(11)6(2-4(3)10)16-7(15)8(12,13)14/h1-2H
InchiKey:	REMBFCXQZGOYLI-UHFFFAOYSA-N
Formula:	C8H2Cl6O2
SMILES:	O=C(Oc1cc(Cl)c(Cl)cc1Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	342.82
CAS:	25438-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-202.66	kJ/mol	Joback Method
hf	-354.32	kJ/mol	Joback Method
hfus	29.91	kJ/mol	Joback Method
hvap	71.83	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.922		Crippen Method
mvol	180.700	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
tb	721.70	K	Joback Method
tc	980.67	K	Joback Method
tf	498.00	K	Joback Method
vc	0.682	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.18	J/molxK	721.70	Joback Method
cpg	341.17	J/molxK	764.86	Joback Method
cpg	346.48	J/molxK	808.02	Joback Method
cpg	351.15	J/molxK	851.19	Joback Method
cpg	355.23	J/molxK	894.35	Joback Method
cpg	358.77	J/molxK	937.51	Joback Method
cpg	361.81	J/molxK	980.67	Joback Method
dvisc	0.0007081	Paxs	498.00	Joback Method
dvisc	0.0004936	Paxs	535.28	Joback Method

dvisc	0.0003607	Paxs	572.57	Joback Method
dvisc	0.0002738	Paxs	609.85	Joback Method
dvisc	0.0002146	Paxs	647.13	Joback Method
dvisc	0.0001727	Paxs	684.42	Joback Method
dvisc	0.0001421	Paxs	721.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25438237&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:

<https://www.chemeo.com/cid/28-075-8/2-4-5-Trichlorophenyl-trichloroacetate.pdf>

Generated by Cheméo on 2024-04-18 02:40:06.062993175 +0000 UTC m=+15697254.983570492.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.