

2,4-Dichlorophenyl trichloroacetate

Inchi:	InChI=1S/C8H3Cl5O2/c9-4-1-2-6(5(10)3-4)15-7(14)8(11,12)13/h1-3H
InchiKey:	VNVHPDIADHUZNF-UHFFFAOYSA-N
Formula:	C8H3Cl5O2
SMILES:	O=C(Oc1ccc(Cl)cc1Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	308.37
CAS:	23399-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-181.10	kJ/mol	Joback Method
hf	-327.11	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	66.79	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.269		Crippen Method
mcvol	168.460	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	679.29	K	Joback Method
tc	935.40	K	Joback Method
tf	455.56	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.65	J/molxK	679.29	Joback Method
cpg	327.75	J/molxK	721.97	Joback Method
cpg	334.09	J/molxK	764.66	Joback Method
cpg	339.73	J/molxK	807.34	Joback Method
cpg	344.71	J/molxK	850.03	Joback Method
cpg	349.09	J/molxK	892.71	Joback Method
cpg	352.92	J/molxK	935.40	Joback Method
dvisc	0.0009686	Paxs	455.56	Joback Method
dvisc	0.0006437	Paxs	492.85	Joback Method

dvisc	0.0004531	Paxs	530.14	Joback Method
dvisc	0.0003340	Paxs	567.42	Joback Method
dvisc	0.0002557	Paxs	604.71	Joback Method
dvisc	0.0002019	Paxs	642.00	Joback Method
dvisc	0.0001636	Paxs	679.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23399817&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
mccvol:	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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