1-(2,4,5-Trichlorophenyl)ethanol

Inchi: InChI=1S/C8H7Cl3O/c1-4(12)5-2-7(10)8(11)3-6(5)9/h2-4,12H,1H3
InchiKey: CZTWWYRPCFIOMY-UHFFFAOYSA-N
Formula: C8H7Cl3O
SMILES: CC(O)c1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 225.50
CAS: 14299-54-8

Physical Properties

Property code	Value	Unit	Source
gf	-75.05	kJ/mol	Joback Method
hf	-211.06	kJ/mol	Joback Method
hfus	22.51	kJ/mol	Joback Method
hvap	67.11	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.700		Crippen Method
mcvol	142.410	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	1556.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	628.09	K	Joback Method
tc	846.04	K	Joback Method
tf	379.48	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.80	J/mol×K	628.09	Joback Method
cpg	295.83	J/mol×K	664.42	Joback Method
cpg	303.35	J/mol×K	700.74	Joback Method
cpg	310.38	J/mol×K	737.07	Joback Method
cpg	316.94	J/mol×K	773.39	Joback Method

cpg	323.04	J/mol×K	809.72	Joback Method
cpg	328.71	J/mol×K	846.04	Joback Method
dvisc	0.0022445	Pa×s	379.48	Joback Method
dvisc	0.0009749	Pa×s	420.92	Joback Method
dvisc	0.0004917	Pa×s	462.35	Joback Method
dvisc	0.0002775	Pa×s	503.79	Joback Method
dvisc	0.0001709	Pa×s	545.22	Joback Method
dvisc	0.0001127	Pa×s	586.65	Joback Method
dvisc	0.0000785	Pa×s	628.09	Joback Method

Sources

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=C14299548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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