1-(2,4,5-trichlorophenyl)-2-chloro-ethanol-1

Inchi: InChI=1S/C8H6Cl4O/c9-3-8(13)4-1-6(11)7(12)2-5(4)10/h1-2,8,13H,3H2
InchiKey: JQMCNRIUQZHIPP-UHFFFAOYSA-N
Formula: C8H6Cl4O
SMILES: OC(CCl)c1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 259.94

Physical Properties

Property code	Value	Unit	Source
gf	-86.98	kJ/mol	Joback Method
hf	-226.80	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	71.49	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.919		Crippen Method
mcvol	154.650	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1723.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1711.00		NIST Webbook
tb	665.52	K	Joback Method
tc	886.77	K	Joback Method
tf	409.40	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.09	J/mol×K	665.52	Joback Method
cpg	314.39	J/mol×K	702.39	Joback Method
cpg	321.18	J/mol×K	739.27	Joback Method
cpg	327.49	J/mol×K	776.14	Joback Method
cpg	333.33	J/mol×K	813.02	Joback Method
cpg	338.73	J/mol×K	849.89	Joback Method

cpg	343.72	J/mol×K	886.77	Joback Method
dvisc	0.0015777	Pa×s	409.40	Joback Method
dvisc	0.0007226	Pa×s	452.09	Joback Method
dvisc	0.0003787	Pa×s	494.77	Joback Method
dvisc	0.0002199	Pa×s	537.46	Joback Method
dvisc	0.0001383	Pa×s	580.15	Joback Method
dvisc	0.0000927	Pa×s	622.83	Joback Method
dvisc	0.0000654	Pa×s	665.52	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R141598&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
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

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