Ethanone, 1-(2,4,5-trichlorophenyl)-

Other names: 1-(2,4,5-trichlorophenyl)ethan-1-one
Inchi: InChI=1S/C8H5Cl3O/c1-4(12)5-2-7(10)8(11)3-6(5)9/h2-3H,1H3
InchiKey: OPPQOJRXXODMKR-UHFFFAOYSA-N
Formula: C8H5Cl3O
SMILES: CC(=O)c1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 223.48
CAS: 13061-28-4

Physical Properties

Property code	Value	Unit	Source
gf	-64.71	kJ/mol	Joback Method
hf	-166.13	kJ/mol	Joback Method
hfus	23.54	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.849		Crippen Method
mcvol	138.110	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1463.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	590.22	K	Joback Method
tc	830.14	K	Joback Method
tf	383.59	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.97	J/mol×K	590.22	Joback Method
cpg	293.51	J/mol×K	790.16	Joback Method
cpg	287.30	J/mol×K	750.17	Joback Method

cpg	280.56	J/mol×K	710.18	Joback Method
cpg	273.28	J/mol×K	670.19	Joback Method
cpg	265.42	J/mol×K	630.21	Joback Method
cpg	299.21	J/mol×K	830.14	Joback Method
dvisc	0.0002821	Pa×s	590.22	Joback Method
dvisc	0.0003373	Pa×s	555.78	Joback Method
dvisc	0.0004130	Pa×s	521.34	Joback Method
dvisc	0.0005204	Pa×s	486.91	Joback Method
dvisc	0.0006791	Pa×s	452.47	Joback Method
dvisc	0.0009261	Pa×s	418.03	Joback Method
dvisc	0.0013352	Pa×s	383.59	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=C13061284&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