[2H7]-2,3,5-Trichloro-1,4-dimethylbenzene

Inchi: InChI=1S/C8H7Cl3/c1-4-3-6(9)5(2)8(11)7(4)10/h3H,1-2H3/i1D3,2D3,3D
InchiKey: VMMUHZZNIYRBPI-YYWVXINBSA-N
Formula: C8D7Cl3
SMILES: Cc1cc(Cl)c(C)c(Cl)c1Cl
Mol. weight [g/mol]: 216.54

Physical Properties

Property code	Value	Unit	Source
gf	54.58	kJ/mol	Joback Method
hf	-65.02	kJ/mol	Joback Method
hfus	21.55	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.264		Crippen Method
mcvol	136.540	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1416.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1416.00		NIST Webbook
tb	541.33	K	Joback Method
tc	774.34	K	Joback Method
tf	346.18	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.37	J/mol×K	541.33	Joback Method
cpg	288.52	J/mol×K	735.50	Joback Method
cpg	281.27	J/mol×K	696.67	Joback Method
cpg	273.54	J/mol×K	657.83	Joback Method
cpg	265.33	J/mol×K	619.00	Joback Method
cpg	256.61	J/mol×K	580.16	Joback Method
cpg	295.30	J/mol×K	774.34	Joback Method

dvisc	0.0002531	Pa×s	541.33	Joback Method
dvisc	0.0002988	Pa×s	508.81	Joback Method
dvisc	0.0003608	Pa×s	476.28	Joback Method
dvisc	0.0004480	Pa×s	443.76	Joback Method
dvisc	0.0005756	Pa×s	411.23	Joback Method
dvisc	0.0007721	Pa×s	378.71	Joback Method
dvisc	0.0010943	Pa×s	346.18	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=R389047&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