1,2,3-Trichloro-4,5,6-trimethylbenzene

Inchi: InChI=1S/C9H9Cl3/c1-4-5(2)7(10)9(12)8(11)6(4)3/h1-3H3
InchiKey: QCTIBRJBUAXXEB-UHFFFAOYSA-N
Formula: C9H9Cl3
SMILES: Cc1c(C)c(Cl)c(Cl)c(Cl)c1C
Mol. weight [g/mol]: 223.53
CAS: 19219-81-9

Physical Properties

Property code	Value	Unit	Source
gf	53.37	kJ/mol	Joback Method
hf	-97.13	kJ/mol	Joback Method
hfus	23.75	kJ/mol	Joback Method
hvap	54.37	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.572		Crippen Method
mcvol	150.630	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
ss	314.93	J/mol×K	NIST Webbook
tb	569.19	K	Joback Method
tc	798.82	K	Joback Method
tf	498.00 ± 2.00	K	NIST Webbook
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.35	J/mol×K	569.19	Joback Method
cpg	299.51	J/mol×K	607.46	Joback Method
cpg	309.13	J/mol×K	645.73	Joback Method
cpg	318.24	J/mol×K	684.00	Joback Method
cpg	326.84	J/mol×K	722.27	Joback Method
cpg	334.94	J/mol×K	760.55	Joback Method
cpg	342.55	J/mol×K	798.82	Joback Method
cps	252.34	J/mol×K	298.15	NIST Webbook

dvisc	0.0009091	Pa×s	369.97	Joback Method
dvisc	0.0006585	Pa×s	403.17	Joback Method
dvisc	0.0005009	Pa×s	436.38	Joback Method
dvisc	0.0003961	Pa×s	469.58	Joback Method
dvisc	0.0003231	Pa×s	502.78	Joback Method
dvisc	0.0002703	Pa×s	535.99	Joback Method
dvisc	0.0002308	Pa×s	569.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19219819&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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