1,1,3-trichlorobutane

Inchi: InChI=1S/C4H7Cl3/c1-3(5)2-4(6)7/h3-4H,2H2,1H3
InchiKey: GSBUVYHAANRCNO-UHFFFAOYSA-N
Formula: C4H7Cl3
SMILES: CC(Cl)CC(Cl)Cl
Mol. weight [g/mol]: 161.46
CAS: 13279-87-3

Physical Properties

Property code	Value	Unit	Source
gf	-57.87	kJ/mol	Joback Method
hf	-183.67	kJ/mol	Joback Method
hfus	11.66	kJ/mol	Joback Method
hvap	36.88	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.807		Crippen Method
mcvol	103.940	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
tb	423.00 ± 4.00	K	NIST Webbook
tb	423.00 ± 3.00	K	NIST Webbook
tc	601.91	K	Joback Method
tf	194.60	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.69	J/mol×K	402.33	Joback Method
cpg	198.08	J/mol×K	568.64	Joback Method
cpg	191.94	J/mol×K	535.38	Joback Method
cpg	185.45	J/mol×K	502.12	Joback Method
cpg	178.58	J/mol×K	468.86	Joback Method
cpg	171.34	J/mol×K	435.59	Joback Method
cpg	203.87	J/mol×K	601.91	Joback Method
dvisc	0.0003596	Pa×s	402.33	Joback Method

dvisc	0.0004848	Pa×s	367.71	Joback Method
dvisc	0.0006955	Pa×s	333.09	Joback Method
dvisc	0.0010849	Pa×s	298.47	Joback Method
dvisc	0.0019018	Pa×s	263.84	Joback Method
dvisc	0.0039497	Pa×s	229.22	Joback Method
dvisc	0.0106392	Pa×s	194.60	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=C13279873&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume