1,1,2-TRICHLORO-2-METHYLPROPANE

Inchi: InChI=1S/C4H7Cl3/c1-4(2,7)3(5)6/h3H,1-2H3
InchiKey: FRRHZKFKOHHEJR-UHFFFAOYSA-N
Formula: C4H7Cl3
SMILES: CC(C)(Cl)C(Cl)Cl
Mol. weight [g/mol]: 161.46

Physical Properties

Property code	Value	Unit	Source
af	0.2636		Cheméo Relay (1.0)
gf	-52.59	kJ/mol	Joback Method
hf	-209.35	kJ/mol	Cheméo Relay (1.0)
hfus	7.77	kJ/mol	Joback Method
hvap	41.99	kJ/mol	Cheméo Relay (1.0)
ie	10.71	eV	Cheméo Relay (1.0)
log10ws	-2.72		Cheméo Relay (1.0)
logp	2.807		Crippen Method
mcvol	103.940	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	869.00		NIST Webbook
tb	407.90	K	Cheméo Relay (1.0)
tc	627.98	K	Cheméo Relay (1.0)
tf	288.63	K	Cheméo Relay (1.0)
vc	0.370	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.86	J/mol×K	399.54	Joback Method
cpg	174.47	J/mol×K	434.30	Joback Method
cpg	182.46	J/mol×K	469.06	Joback Method
cpg	189.88	J/mol×K	503.81	Joback Method
cpg	196.74	J/mol×K	538.57	Joback Method
cpg	203.10	J/mol×K	573.33	Joback Method
cpg	208.98	J/mol×K	608.09	Joback Method

dvisc	0.0108227	Pa×s	212.02	Joback Method
dvisc	0.0044160	Pa×s	243.27	Joback Method
dvisc	0.0022098	Pa×s	274.53	Joback Method
dvisc	0.0012740	Pa×s	305.78	Joback Method
dvisc	0.0008134	Pa×s	337.03	Joback Method
dvisc	0.0005605	Pa×s	368.29	Joback Method
dvisc	0.0004093	Pa×s	399.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29559522&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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