2,2,2-Trichloroethanol, trifluoroacetate

Other names: 2,2,2-Trichloroethanol, trifluoroacetate
Inchi: InChI=1S/C4H2Cl3F3O2/c5-3(6,7)1-12-2(11)4(8,9)10/h1H2
InchiKey: BGZNVJXNPFAPCN-UHFFFAOYSA-N
Formula: C4H2Cl3F3O2
SMILES: O=C(OCC(Cl)(Cl)Cl)C(F)(F)F
Mol. weight [g/mol]: 245.41

Physical Properties

Property code	Value	Unit	Source
hf	-1039.02	kJ/mol	Cheméo Relay (1.0)
hfus	15.91	kJ/mol	Joback Method
hvap	49.52	kJ/mol	Cheméo Relay (1.0)
ie	11.66	eV	Cheméo Relay (1.0)
logp	2.462		Crippen Method
mcvol	116.690	ml/mol	McGowan Method
rinpol	823.00		NIST Webbook
tb	412.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.48	J/mol×K	470.85	Joback Method
cpg	231.27	J/mol×K	503.29	Joback Method
cpg	237.48	J/mol×K	535.73	Joback Method
cpg	243.14	J/mol×K	568.18	Joback Method
cpg	248.28	J/mol×K	600.62	Joback Method
cpg	252.94	J/mol×K	633.06	Joback Method
cpg	257.16	J/mol×K	665.50	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=C153654718&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature