2,2,2-Trichloroethyl 2,2,2-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
CAS: 153654-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-865.66	kJ/mol	Joback Method
hf	-1023.74	kJ/mol	Joback Method
hfus	15.91	kJ/mol	Joback Method
hvap	41.77	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.462		Crippen Method
mcvol	116.690	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	823.00		NIST Webbook
tb	470.85	K	Joback Method
tc	665.50	K	Joback Method
tf	303.37	K	Joback Method
vc	0.463	m3/kmol	Joback Method

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

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=C153654718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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