2,2,2-Trichloroethanol, pentafluoropropionate

Inchi: InChI=1S/C5H2Cl3F5O2/c6-3(7,8)1-15-2(14)4(9,10)5(11,12)13/h1H2
InchiKey: OSKSLSQEVUZXAC-UHFFFAOYSA-N
Formula: C5H2Cl3F5O2
SMILES: O=C(OCC(Cl)(Cl)Cl)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 295.42

Physical Properties

Property code	Value	Unit	Source
gf	-1244.02	kJ/mol	Joback Method
hf	-1445.35	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	41.06	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.097		Crippen Method
mcvol	134.320	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	854.00		NIST Webbook
tb	489.04	K	Joback Method
tc	673.81	K	Joback Method
tf	318.24	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.85	J/mol×K	489.04	Joback Method
cpg	291.71	J/mol×K	519.83	Joback Method
cpg	298.85	J/mol×K	550.63	Joback Method
cpg	305.32	J/mol×K	581.42	Joback Method
cpg	311.15	J/mol×K	612.22	Joback Method
cpg	316.41	J/mol×K	643.01	Joback Method
cpg	321.12	J/mol×K	673.81	Joback Method

Sources

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=U375580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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