Propane, 1,1,1,2,2,3-hexachloro-3,3-difluoro-

Other names: 1,1-Difluoro-1,2,2,3,3,3-hexachloro propane
Inchi: InChI=1S/C3Cl6F2/c4-1(5,2(6,7)8)3(9,10)11
InchiKey: NKPXIDLSGFFJOI-UHFFFAOYSA-N
Formula: C3Cl6F2
SMILES: FC(F)(Cl)C(Cl)(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 286.75
CAS: 661-96-1

Physical Properties

Property code	Value	Unit	Source
gf	-478.30	kJ/mol	Joback Method
hf	-618.16	kJ/mol	Joback Method
hfus	12.63	kJ/mol	Joback Method
hvap	43.06	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.362		Crippen Method
mcvol	130.110	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	481.47	K	Joback Method
tc	713.79	K	Joback Method
tf	324.00 ± 1.00	K	NIST Webbook
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.35	J/mol×K	481.47	Joback Method
cpg	220.13	J/mol×K	520.19	Joback Method
cpg	224.90	J/mol×K	558.91	Joback Method
cpg	228.79	J/mol×K	597.63	Joback Method
cpg	231.88	J/mol×K	636.35	Joback Method
cpg	234.30	J/mol×K	675.07	Joback Method
cpg	236.14	J/mol×K	713.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C661961&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume