1,2-Dibromohexafluoropropane

Other names: Propane, 1,2-dibromo-1,1,2,3,3,3-hexafluoro-
1,2-Dibromo-1,1,2,3,3,3-hexafluoropropane
Inchi: InChI=1S/C3Br2F6/c4-1(6,2(5,7)8)3(9,10)11
InchiKey: KTULQNFKNLFOHL-UHFFFAOYSA-N
Formula: C3Br2F6
SMILES: FC(F)(F)C(F)(Br)C(F)(F)Br
Mol. weight [g/mol]: 309.83
CAS: 661-95-0

Physical Properties

Property code	Value	Unit	Source
gf	-1157.32	kJ/mol	Joback Method
hf	-1255.50	kJ/mol	Joback Method
hfus	10.33	kJ/mol	Joback Method
hvap	26.35	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.597		Crippen Method
mcvol	98.750	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	345.90	K	NIST Webbook
tc	567.66	K	Joback Method
tf	253.97	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.89	J/mol×K	386.29	Joback Method
cpg	187.73	J/mol×K	416.52	Joback Method
cpg	194.72	J/mol×K	446.75	Joback Method
cpg	200.91	J/mol×K	476.97	Joback Method
cpg	206.35	J/mol×K	507.20	Joback Method
cpg	211.11	J/mol×K	537.43	Joback Method
cpg	215.24	J/mol×K	567.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.20	K	97.90	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C661950&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume