1,2-Dibromo-1,1,2,3,3,3,-hexafluoropropane

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

Physical Properties

Property code	Value	Unit	Source
af	0.3600		Cheméo Relay (1.0)
hf	-1277.45	kJ/mol	Cheméo Relay (1.0)
hfus	10.33	kJ/mol	Joback Method
hvap	30.86	kJ/mol	Cheméo Relay (1.0)
ie	11.31	eV	Cheméo Relay (1.0)
logp	3.597		Crippen Method
mcvol	98.750	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	342.88	K	Cheméo Relay (1.0)
tc	491.13	K	Cheméo Relay (1.0)
tf	131.17	K	Cheméo Relay (1.0)
vc	0.382	m3/kmol	Cheméo Relay (1.0)

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

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C661950&Units=SI

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume