1,6-Dibromo-2,3,5-trichlorononafluorohexane

Inchi: InChI=1S/C6Br2Cl3F9/c7-5(17,18)2(10,13)1(9,12)4(15,16)3(11,14)6(8,19)20
InchiKey: RKKGNUHLABLELO-UHFFFAOYSA-N
Formula: C6Br2Cl3F9
SMILES: FC(F)(Br)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(Cl)C(F)(F)Br
Mol. weight [g/mol]: 509.22
CAS: 85131-86-8

Physical Properties

Property code	Value	Unit	Source
gf	-1743.76	kJ/mol	Joback Method
hf	-1979.22	kJ/mol	Joback Method
hfus	17.69	kJ/mol	Joback Method
hvap	39.85	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.311		Crippen Method
mcvol	183.050	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
tb	555.34	K	Joback Method
tc	754.56	K	Joback Method
tf	386.57	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.50	J/mol×K	555.34	Joback Method
cpg	408.13	J/mol×K	588.54	Joback Method
cpg	414.52	J/mol×K	621.75	Joback Method
cpg	419.81	J/mol×K	654.95	Joback Method
cpg	424.16	J/mol×K	688.15	Joback Method
cpg	427.68	J/mol×K	721.36	Joback Method
cpg	430.53	J/mol×K	754.56	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=C85131868&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume