1,4-Dibromo-2,3-dichlorohexafluorobutane

Inchi: InChI=1S/C4Br2Cl2F6/c5-3(11,12)1(7,9)2(8,10)4(6,13)14
InchiKey: PFSLUJSDDNGKIZ-UHFFFAOYSA-N
Formula: C4Br2Cl2F6
SMILES: FC(F)(Br)C(F)(Cl)C(F)(Cl)C(F)(F)Br
Mol. weight [g/mol]: 392.75
CAS: 375-42-8

Physical Properties

Property code	Value	Unit	Source
gf	-1169.92	kJ/mol	Joback Method
hf	-1316.37	kJ/mol	Joback Method
hfus	13.90	kJ/mol	Joback Method
hvap	36.05	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.771		Crippen Method
mcvol	137.320	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	480.80	K	Joback Method
tc	686.68	K	Joback Method
tf	327.50	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.69	J/mol×K	583.74	Joback Method
cpg	288.19	J/mol×K	618.05	Joback Method
cpg	291.88	J/mol×K	652.36	Joback Method
cpg	264.33	J/mol×K	480.80	Joback Method
cpg	271.87	J/mol×K	515.11	Joback Method
cpg	278.29	J/mol×K	549.43	Joback Method
cpg	294.88	J/mol×K	686.68	Joback Method
cpl	298.50	J/mol×K	298.16	NIST Webbook
hvapt	47.70 ± 0.10	kJ/mol	308.00	NIST Webbook

hvapt	46.90 ± 0.10	kJ/mol	315.00	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=C375428&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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