Hexane, 1,6-dibromo-dodecafluoro-

Inchi: InChI=1S/C6Br2F12/c7-5(17,18)3(13,14)1(9,10)2(11,12)4(15,16)6(8,19)20
InchiKey: SWAPKQWKFYIOJS-UHFFFAOYSA-N
Formula: C6Br2F12
SMILES: FC(F)(Br)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br
Mol. weight [g/mol]: 459.85
CAS: 918-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-2292.40	kJ/mol	Joback Method
hf	-2520.33	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	24.24	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.503		Crippen Method
mcvol	151.640	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
tb	440.86	K	Joback Method
tc	598.18	K	Joback Method
tf	298.58	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.47	J/mol×K	440.86	Joback Method
cpg	361.36	J/mol×K	467.08	Joback Method
cpg	371.16	J/mol×K	493.30	Joback Method
cpg	379.93	J/mol×K	519.52	Joback Method
cpg	387.75	J/mol×K	545.74	Joback Method
cpg	394.68	J/mol×K	571.96	Joback Method
cpg	400.79	J/mol×K	598.18	Joback Method

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=C918229&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume