Perfluorobicyclo-[4.4.0]-dec-1,6-ene

Inchi: InChI=1S/C10F16/c11-3(12)1-2(5(15,16)9(23,24)7(3,19)20)6(17,18)10(25,26)8(21,22)4(1
InchiKey: LSBZKGFVMTVTCT-UHFFFAOYSA-N
Formula: C10F16
SMILES: FC1(F)C2=C(C(F)(F)C(F)(F)C1(F)F)C(F)(F)C(F)(F)C(F)(F)C2(F)F
Mol. weight [g/mol]: 424.08
CAS: 54939-04-7

Physical Properties

Property code	Value	Unit	Source
chl	-3550.20 ± 4.60	kJ/mol	NIST Webbook
gf	-3090.02	kJ/mol	Joback Method
hf	-3203.60 ± 4.80	kJ/mol	NIST Webbook
hfl	-3248.70 ± 4.80	kJ/mol	NIST Webbook
hfus	15.29	kJ/mol	Joback Method
hvap	45.30 ± 0.10	kJ/mol	NIST Webbook
log10ws	-6.16		Crippen Method
logp	5.393		Crippen Method
mcvol	154.060	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
sl	491.20	J/mol×K	NIST Webbook
tb	430.10	K	Joback Method
tc	567.49	K	Joback Method
tf	425.26	K	Joback Method
tt	264.09 ± 0.02	K	NIST Webbook
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.68	J/mol×K	544.59	Joback Method
cpg	410.94	J/mol×K	430.10	Joback Method
cpg	424.27	J/mol×K	453.00	Joback Method
cpg	436.04	J/mol×K	475.90	Joback Method
cpg	446.41	J/mol×K	498.79	Joback Method

cpg	455.57	J/mol×K	521.69	Joback Method
cpg	470.94	J/mol×K	567.49	Joback Method
cpl	428.40	J/mol×K	298.15	NIST Webbook
hfust	10.47	kJ/mol	263.00	NIST Webbook

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=C54939047&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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