

Perfluorohexamethyl dewar benzene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C12F18/c13-7(14,15)1-2(8(16,17)18)6(12(28,29)30)4(10(22,23)24)3(9(19,20)21)5(11,25,26,27)F

UHFLOEPBRVWBKP-UHFFFAOYSA-N

C12F18

FC(F)(F)C1=C(C(F)(F)F)C2(C(F)(F)F)C(C(F)(F)F)=C(C(F)(F)F)C12C(F)(F)F

486.10

23174-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-3307.46	kJ/mol	Joback Method
hf	-3627.73	kJ/mol	Joback Method
hfus	22.35	kJ/mol	Joback Method
hvap	20.58	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	6.953		Crippen Method
mcvol	181.480	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
tb	473.64	K	Joback Method
tc	602.97	K	Joback Method
tf	385.42	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.41	J/mol×K	473.64	Joback Method
cpg	527.07	J/mol×K	495.19	Joback Method
cpg	537.67	J/mol×K	516.75	Joback Method
cpg	547.30	J/mol×K	538.30	Joback Method
cpg	556.04	J/mol×K	559.86	Joback Method
cpg	563.97	J/mol×K	581.41	Joback Method
cpg	571.18	J/mol×K	602.97	Joback Method
hvapt	41.40	kJ/mol	318.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23174552&Units=SI
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

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
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

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