Perfluoro-1-methyldecalin

Other names:	Naphthalene, 1,1,2,2,3,3,4,4,4a,5,5,6,6,7,7,8,8a-heptadecafluorodecahydro-8-(trifluoromethyl)-Heptadecafluorodecahydro-1-(trifluoromethyl)naphthalene
	Flutec PP9
	Perfluoro-1-methyldecaline
	Perfluoromethyldecalin
	1,1,2,2,3,3,4,4,4a,5,5,6,6,7,7,8,8a-heptadecafluorodecahydro-8-(trifluoromethyl)naphthal
Inchi:	InChI=1S/C11F20/c12-1-2(13,6(19,20)10(27,28)9(25,26)4(1,15)16)5(17,18)8(23,24)7(21
InchiKey:	LWRNQOBXRHWPGE-UHFFFAOYSA-N
Formula:	C11F20
SMILES:	FC(F)(F)C1(F)C(F)(F)C(F)(F)C(F)(F)C2(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C12F
Mol. weight [g/mol]:	512.09
CAS:	306-92-3

Physical Properties

Property code	Value	Unit	Source
gf	-3895.10	kJ/mol	Joback Method
hf	-4090.68	kJ/mol	Joback Method
hfus	11.89	kJ/mol	Joback Method
hvap	8.98	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.148		Crippen Method
mcvol	179.530	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
tb	432.50 ± 0.50	K	NIST Webbook
tc	555.54	K	Joback Method
tf	454.83	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.62	J/mol×K	428.85	Joback Method
cpg	516.23	J/mol×K	449.97	Joback Method
cpg	530.07	J/mol×K	471.08	Joback Method

cpg	542.33	J/mol×K	492.20	Joback Method
cpg	553.18	J/mol×K	513.31	Joback Method
cpg	562.80	J/mol×K	534.43	Joback Method
cpg	571.36	J/mol×K	555.54	Joback Method

Sources

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=C306923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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