

Perfluoro-1,3-dimethylcyclohexane

Other names:	1,1,2,2,3,3,4,5,5,6-decafluoro-4,6-bis(trifluoromethyl)cyclohexane Cyclohexane, perfluoro-1,3-dimethyl- FLUTEC PP3102 Flutec PP3 cyclohexane, 1,1,2,2,3,3,4,5,5,6-decafluoro-4,6-bis(trifluoromethyl)- cyclohexane, decafluoro-1,3-bis(trifluoromethyl)- decafluoro-1,3-bis(trifluoromethyl)cyclohexane flutec PP 3 perfluoro(1,3-dimethylcyclohexane) perfluoro-m-dimethylcyclohexane
Inchi:	InChI=1S/C8F16/c9-1(7(19,20)21)3(11,12)2(10,8(22,23)24)5(15,16)6(17,18)4(1,13)14
InchiKey:	LOQGSOTUHASIHI-UHFFFAOYSA-N
Formula:	C8F16
SMILES:	FC(F)(F)C1(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C1(F)F
Mol. weight [g/mol]:	400.06
CAS:	335-27-3

Physical Properties

Property code	Value	Unit	Source
gf	-3141.84	kJ/mol	Joback Method
hf	-3319.65	kJ/mol	Joback Method
hfus	10.33	kJ/mol	Joback Method
hvap	9.72	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.082		Crippen Method
mcvol	141.040	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	462.00		NIST Webbook
rinpol	462.00		NIST Webbook
tb	374.50 ± 0.50	K	NIST Webbook
tc	485.25	K	Joback Method
tf	323.78	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.62	J/mol×K	361.94	Joback Method
cpg	357.56	J/mol×K	382.49	Joback Method
cpg	372.02	J/mol×K	403.04	Joback Method
cpg	385.10	J/mol×K	423.59	Joback Method
cpg	396.90	J/mol×K	444.14	Joback Method
cpg	407.54	J/mol×K	464.69	Joback Method
cpg	417.10	J/mol×K	485.25	Joback Method
hvapt	37.40	kJ/mol	341.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C335273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental data on binary and ternary mixtures of perfluorooctane with hexane with	https://www.doi.org/10.1016/j.fluid.2010.06.017
thermodynamics and solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids:	https://www.doi.org/10.1016/j.jct.2006.11.012
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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

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