Perfluorotributylamine

Other names:
(n-C4F9)3N
1-Butanamine, 1,1,2,2,3,3,4,4,4-nonafluoro-N,N-bis(1,1,2,2,3,3,4,4,4-nonafluorobutyl)-
1-Butanamine, 1,1,2,2,3,3,4,4,4-nonafluoro-N,N-bis(nonafluorobutyl)-
Butylamine, 1,1,2,2,3,3,4,4,4-nonafluoro-N,N-bis(nonafluorobutyl)-
FC 43
FC 47
Fluorinert FC 43
Fluorocarbon FC 43
Fluosol 43
Heptacosafluorotri-n-butylamine
Heptacosafluorotributylamine
Mediflor FC 43
Medifluor FC 47
NSC 3501
PFTBA
Perfluorotri-n-butylamine
Tri(nonafluorobutyl)amine
Tributylamine, heptacosafluoro-
Tris(nonafluorobutyl)amine
Tris(perfluorobutyl)amine
tri(Perfluorobutyl)amine

Inchi: InChI=1S/C12F27N/c13-1(14,7(25,26)27)4(19,20)10(34,35)40(11(36,37)5(21,22)2(15,16
InchiKey: RVZRBWKZFJCCIB-UHFFFAOYSA-N
Formula: C12F27N
SMILES: FC(F)(F)C(F)(F)C(F)(F)C(F)(F)N(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C
Mol. weight [g/mol]: 671.09
CAS: 311-89-7

Physical Properties

Property code	Value	Unit	Source
chl	-3852.00 ± 9.20	kJ/mol	NIST Webbook
gf	-5064.85	kJ/mol	Joback Method
hf	-5583.50	kJ/mol	NIST Webbook
hfl	-5643.80	kJ/mol	NIST Webbook
hfus	24.05	kJ/mol	Joback Method
hvap	60.30 ± 0.10	kJ/mol	NIST Webbook

hvap	60.40 ± 1.20	kJ/mol	NIST Webbook
hvap	60.40 ± 1.20	kJ/mol	NIST Webbook
ie	11.30	eV	NIST Webbook
ie	11.70	eV	NIST Webbook
ie	11.30	eV	NIST Webbook
log10ws	-9.71		Crippen Method
logp	8.566		Crippen Method
mcvol	237.710	ml/mol	McGowan Method
pc	886.30	kPa	Joback Method
tb	451.00	K	NIST Webbook
tb	452.20	K	NIST Webbook
tb	451.95 ± 1.00	K	NIST Webbook
tc	528.64	K	Joback Method
tf	302.44	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.72	J/mol×K	495.07	Joback Method
cpg	744.93	J/mol×K	511.85	Joback Method
cpg	675.18	J/mol×K	427.93	Joback Method
cpg	690.94	J/mol×K	444.71	Joback Method
cpg	705.77	J/mol×K	461.50	Joback Method
cpg	719.68	J/mol×K	478.28	Joback Method
cpg	756.33	J/mol×K	528.64	Joback Method
hvapt	57.40	kJ/mol	374.00	NIST Webbook
hvapt	51.10	kJ/mol	457.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50242e+01
Coeff. B	-3.87093e+03
Coeff. C	-7.91550e+01
Temperature range (K), min.	341.83

Temperature range (K), max.	477.70

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=C311897&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume