

t-Butyldifluoroamine

Inchi:	InChI=1S/C4H9F2N/c1-4(2,3)7(5)6/h1-3H3
InchiKey:	LXLQMSOUIOCFMO-UHFFFAOYSA-N
Formula:	C4H9F2N
SMILES:	CC(C)(C)N(F)F
Mol. weight [g/mol]:	109.12
CAS:	646-55-9

Physical Properties

Property code	Value	Unit	Source
chl	-2986.00 ± 3.00	kJ/mol	NIST Webbook
gf	-293.20	kJ/mol	Joback Method
hf	-192.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-221.00 ± 3.00	kJ/mol	NIST Webbook
hfus	7.88	kJ/mol	Joback Method
hvap	29.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-1.87		Crippen Method
logp	1.856		Crippen Method
mcvol	80.740	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	298.67	K	Joback Method
tc	451.67	K	Joback Method
tf	170.91	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.14	J/mol×K	298.67	Joback Method
cpg	140.95	J/mol×K	324.17	Joback Method
cpg	150.29	J/mol×K	349.67	Joback Method
cpg	159.18	J/mol×K	375.17	Joback Method
cpg	167.63	J/mol×K	400.67	Joback Method
cpg	175.67	J/mol×K	426.17	Joback Method
cpg	183.30	J/mol×K	451.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C646559&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

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
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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