Trifluoroacetamide, n-butyl-N-phenyl-

Other names: N-Butylaniline, TFA
Inchi: InChI=1S/C12H14F3NO/c1-2-3-9-16(11(17)12(13,14)15)10-7-5-4-6-8-10/h4-8H,2-3,9H2,
InchiKey: NPRVYZWJDSWWJG-UHFFFAOYSA-N
Formula: C12H14F3NO
SMILES: CCCCN(C(=O)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]: 245.24

Physical Properties

Property code	Value	Unit	Source
gf	-437.16	kJ/mol	Joback Method
hf	-696.61	kJ/mol	Joback Method
hfus	27.32	kJ/mol	Joback Method
hvap	49.62	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.382		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
tb	561.53	K	Joback Method
tc	750.28	K	Joback Method
tf	338.01	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.97	J/mol×K	561.53	Joback Method
cpg	446.77	J/mol×K	592.99	Joback Method
cpg	460.61	J/mol×K	624.45	Joback Method
cpg	473.53	J/mol×K	655.91	Joback Method
cpg	485.58	J/mol×K	687.37	Joback Method
cpg	496.83	J/mol×K	718.82	Joback Method
cpg	507.32	J/mol×K	750.28	Joback Method

Sources

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=U328351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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