Trifluoroacetamide, N-phenyl-n-propyl-

Other names: N-Propylaniline, TFA
Inchi: InChI=1S/C11H12F3NO/c1-2-8-15(10(16)11(12,13)14)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey: FSMYTXOWWYDVRT-UHFFFAOYSA-N
Formula: C11H12F3NO
SMILES: CCCN(C(=O)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]: 231.21

Physical Properties

Property code	Value	Unit	Source
gf	-445.58	kJ/mol	Joback Method
hf	-675.97	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	47.40	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.992		Crippen Method
mcvol	158.950	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
tb	538.65	K	Joback Method
tc	729.70	K	Joback Method
tf	326.74	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.24	J/mol×K	538.65	Joback Method
cpg	398.50	J/mol×K	570.49	Joback Method
cpg	411.80	J/mol×K	602.33	Joback Method
cpg	424.20	J/mol×K	634.17	Joback Method
cpg	435.74	J/mol×K	666.02	Joback Method
cpg	446.48	J/mol×K	697.86	Joback Method
cpg	456.47	J/mol×K	729.70	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=U328350&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