Acetamide, 2,2,2-trifluoro-N-phenyl-

Other names: Acetanilide, 2,2,2-trifluoro-
«alpha»,«alpha»,«alpha»-Trifluoroacetanilide
2,2,2-Trifluoroacetanilide
Alpha,alpha,alpha-trifluoroacetanilide
Trifluoroacetamide, N-phenyl
2,2,2-trifluoro-N-phenylacetamide

Inchi: InChI=1S/C8H6F3NO/c9-8(10,11)7(13)12-6-4-2-1-3-5-6/h1-5H,(H,12,13)

InchiKey: SAPQIENQEZURNZ-UHFFFAOYSA-N

Formula: C8H6F3NO

SMILES: O=C(Nc1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 189.13

CAS: 404-24-0

Physical Properties

Property code	Value	Unit	Source
gf	-492.23	kJ/mol	Joback Method
hf	-628.11	kJ/mol	Joback Method
hfus	19.04	kJ/mol	Joback Method
hvap	45.11	kJ/mol	Joback Method
ie	8.93 ± 0.05	eV	NIST Webbook
log10ws	-2.34		Crippen Method
logp	2.187		Crippen Method
mcvol	116.680	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	193.85		NIST Webbook
tb	507.74	K	Joback Method
tc	710.53	K	Joback Method
tf	313.12	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.08	J/mol×K	507.74	Joback Method

cpg	274.29	J/mol×K	541.54	Joback Method
cpg	284.65	J/mol×K	575.34	Joback Method
cpg	294.22	J/mol×K	609.13	Joback Method
cpg	303.03	J/mol×K	642.93	Joback Method
cpg	311.14	J/mol×K	676.73	Joback Method
cpg	318.59	J/mol×K	710.53	Joback Method

Sources

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=C404240&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
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