N-Trifluoroacetyl-phentermine

Other names:	Phentermine N-TFA
	Phentermine TFA
Inchi:	InChI=1S/C12H14F3NO/c1-11(2,16-10(17)12(13,14)15)8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3
InchiKey:	PRARTRNWRNYCID-UHFFFAOYSA-N
Formula:	C12H14F3NO
SMILES:	CC(C)(Cc1ccccc1)NC(=O)C(F)(F)F
Mol. weight [g/mol]:	245.24
CAS:	42524-63-0

Physical Properties

Property code	Value	Unit	Source
gf	-455.71	kJ/mol	Joback Method
hf	-719.42	kJ/mol	Joback Method
hfus	21.99	kJ/mol	Joback Method
hvap	52.72	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.686		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	596.03	K	Joback Method
tc	798.86	K	Joback Method
tf	360.62	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.95	J/mol×K	596.03	Joback Method
cpg	465.57	J/mol×K	629.83	Joback Method
cpg	479.09	J/mol×K	663.64	Joback Method
cpg	491.59	J/mol×K	697.44	Joback Method
cpg	503.14	J/mol×K	731.25	Joback Method
cpg	513.82	J/mol×K	765.05	Joback Method
cpg	523.70	J/mol×K	798.86	Joback Method

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=C42524630&Units=SI

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