Amphetamine TFA

Other names:	N-Trifluoroacetyl amphetamine
	Amphetamine N-TFA
Inchi:	InChI=1S/C11H12F3NO/c1-8(15-10(16)11(12,13)14)7-9-5-3-2-4-6-9/h2-6,8H,7H2,1H3,(H
InchiKey:	DMOCTORDHSLHLA-UHFFFAOYSA-N
Formula:	C11H12F3NO
SMILES:	CC(Cc1ccccc1)NC(=O)C(F)(F)F
Mol. weight [g/mol]:	231.21

Physical Properties

Property code	Value	Unit	Source
gf	-469.41	kJ/mol	Joback Method
hf	-695.31	kJ/mol	Joback Method
hfus	23.29	kJ/mol	Joback Method
hvap	51.40	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.296		Crippen Method
mcvol	158.950	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
tb	575.94	K	Joback Method
tc	774.38	K	Joback Method
tf	331.93	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.50	J/mol×K	575.94	Joback Method
cpg	413.18	J/mol×K	609.01	Joback Method
cpg	425.92	J/mol×K	642.09	Joback Method
cpg	437.77	J/mol×K	675.16	Joback Method
cpg	448.78	J/mol×K	708.23	Joback Method
cpg	458.99	J/mol×K	741.31	Joback Method

cpg	468.47	J/mol×K	774.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U120307&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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