

2,2,2-Trifluoro-N-[2-[(2,2,2-trifluoroacetyl)amino]p

Inchi:	InChI=1S/C10H6F6N2O2/c11-9(12,13)7(19)17-5-3-1-2-4-6(5)18-8(20)10(14,15)16/h1-4H
InchiKey:	FPBBQCMIENMBEO-UHFFFAOYSA-N
Formula:	C10H6F6N2O2
SMILES:	O=C(Nc1ccccc1NC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	300.16
CAS:	14818-62-3

Physical Properties

Property code	Value	Unit	Source
gf	-1106.14	kJ/mol	Joback Method
hf	-1337.05	kJ/mol	Joback Method
hfus	32.36	kJ/mol	Joback Method
hvap	59.66	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.688		Crippen Method
mcvol	161.720	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1418.00		NIST Webbook
tb	657.10	K	Joback Method
tc	848.61	K	Joback Method
tf	454.96	K	Joback Method
vc	0.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.19	J/molxK	657.10	Joback Method
cpg	450.74	J/molxK	689.02	Joback Method
cpg	459.50	J/molxK	720.94	Joback Method
cpg	467.52	J/molxK	752.85	Joback Method
cpg	474.85	J/molxK	784.77	Joback Method
cpg	481.57	J/molxK	816.69	Joback Method
cpg	487.71	J/molxK	848.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14818623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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