2,2,2-Trifluoro-N-[4-[(2,2,2-trifluoroacetyl)amino]p

Inchi: InChI=1S/C10H6F6N2O2/c11-9(12,13)7(19)17-5-1-2-6(4-3-5)18-8(20)10(14,15)16/h1-4H
InchiKey: IRUADIGSCKQVHY-UHFFFAOYSA-N
Formula: C10H6F6N2O2
SMILES: O=C(Nc1ccc(NC(=O)C(F)(F)F)cc1)C(F)(F)F
Mol. weight [g/mol]: 300.16

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	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	657.10	K	Joback Method
tc	848.61	K	Joback Method
tf	454.96	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373087&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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