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

Inchi: InChI=1S/C12H10F6N2O2/c13-11(14,15)9(21)19-5-7-1-2-8(4-3-7)6-20-10(22)12(16,17)1
InchiKey: WCEYYOFWEXSSQI-UHFFFAOYSA-N
Formula: C12H10F6N2O2
SMILES: O=C(NCc1ccc(CNC(=O)C(F)(F)F)cc1)C(F)(F)F
Mol. weight [g/mol]: 328.21

Physical Properties

Property code	Value	Unit	Source
gf	-1089.30	kJ/mol	Joback Method
hf	-1378.33	kJ/mol	Joback Method
hfus	37.54	kJ/mol	Joback Method
hvap	64.11	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	2.044		Crippen Method
mcvol	189.900	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	1827.00		NIST Webbook
tb	702.86	K	Joback Method
tc	891.41	K	Joback Method
tf	477.50	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.88	J/mol×K	702.86	Joback Method
cpg	551.40	J/mol×K	734.28	Joback Method
cpg	561.11	J/mol×K	765.71	Joback Method
cpg	570.08	J/mol×K	797.13	Joback Method
cpg	578.37	J/mol×K	828.56	Joback Method
cpg	586.03	J/mol×K	859.98	Joback Method
cpg	593.12	J/mol×K	891.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372968&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