2,2,2-Trifluoro-N-bis[2-[(2,2,2-trifluoroacetyl)amino

Other names: 2,2,2-Trifluoro-N-(2,2,2-trifluoroacetyl)-N-[2-(2,2,2-trifluoroacetyl)amino-phenyl]acetamide
Inchi: InChI=1S/C12H5F9N2O3/c13-10(14,15)7(24)22-5-3-1-2-4-6(5)23(8(25)11(16,17)18)9(26
InchiKey: ZGQFSOLLFPTBAK-UHFFFAOYSA-N
Formula: C12H5F9N2O3
SMILES: O=C(Nc1ccccc1N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 396.17

Physical Properties

Property code	Value	Unit	Source
gf	-1778.42	kJ/mol	Joback Method
hf	-2073.93	kJ/mol	Joback Method
hfus	38.88	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.172		Crippen Method
mcvol	196.780	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
tb	713.58	K	Joback Method
tc	895.32	K	Joback Method
tf	511.43	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.44	J/mol×K	713.58	Joback Method
cpg	577.19	J/mol×K	743.87	Joback Method
cpg	585.16	J/mol×K	774.16	Joback Method
cpg	592.42	J/mol×K	804.45	Joback Method
cpg	599.03	J/mol×K	834.74	Joback Method
cpg	605.07	J/mol×K	865.03	Joback Method

cpg	610.61	J/mol×K	895.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378225&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