[2-[(2,2,2-Trifluoroacetyl)amino]phenyl] 2,2,2-trifluoroacetate

Inchi: InChI=1S/C10H5F6NO3/c11-9(12,13)7(18)17-5-3-1-2-4-6(5)20-8(19)10(14,15)16/h1-4H,

InchiKey: ICPWEITZBYZJJN-UHFFFAOYSA-N

Formula: C10H5F6NO3

SMILES: O=C(Nc1ccccc1OC(=O)C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 301.14

Physical Properties

Property code	Value	Unit	Source
gf	-1300.53	kJ/mol	Joback Method
hf	-1522.74	kJ/mol	Joback Method
hfus	28.45	kJ/mol	Joback Method
hvap	55.64	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.655		Crippen Method
mcvol	157.610	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1141.00		NIST Webbook
tb	629.35	K	Joback Method
tc	818.47	K	Joback Method
tf	424.53	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.12	J/mol×K	629.35	Joback Method
cpg	427.81	J/mol×K	660.87	Joback Method
cpg	436.73	J/mol×K	692.39	Joback Method
cpg	444.94	J/mol×K	723.91	Joback Method
cpg	452.47	J/mol×K	755.43	Joback Method
cpg	459.36	J/mol×K	786.95	Joback Method
cpg	465.65	J/mol×K	818.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373046&Units=SI

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