3-CF3-C6H4CONH2

Other names: 3-CF3-C6H4CONH2
Inchi: InChI=1S/C8H6F3NO/c9-8(10,11)6-3-1-2-5(4-6)7(12)13/h1-4H,(H2,12,13)
InchiKey: XBGXGCOLWCMVOI-UHFFFAOYSA-N
Formula: C8H6F3NO
SMILES: NC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 189.14

Physical Properties

Property code	Value	Unit	Source
affp	866.90	kJ/mol	NIST Webbook
basg	836.00	kJ/mol	NIST Webbook
hf	-787.27	kJ/mol	Cheméo Relay (1.0)
hfus	18.75	kJ/mol	Joback Method
hvap	62.18	kJ/mol	Cheméo Relay (1.0)
ie	9.95	eV	Cheméo Relay (1.0)
log10ws	-2.52		Cheméo Relay (1.0)
logp	1.804		Crippen Method
mcvol	116.680	ml/mol	McGowan Method
tb	499.50	K	Cheméo Relay (1.0)
tf	343.50	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.67	J/mol×K	535.08	Joback Method
cpg	282.12	J/mol×K	570.60	Joback Method
cpg	291.77	J/mol×K	606.11	Joback Method
cpg	300.65	J/mol×K	641.63	Joback Method
cpg	308.81	J/mol×K	677.15	Joback Method
cpg	316.31	J/mol×K	712.67	Joback Method
cpg	323.18	J/mol×K	748.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1801101&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point