4-(Trifluoromethoxy)benzamide

Inchi: InChI=1S/C8H6F3NO2/c9-8(10,11)14-6-3-1-5(2-4-6)7(12)13/h1-4H,(H2,12,13)
InchiKey: IDIXWLCRJFBQJA-UHFFFAOYSA-N
Formula: C8H6F3NO2
SMILES: NC(=O)c1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 205.13

Physical Properties

Property code	Value	Unit	Source
hf	-968.37	kJ/mol	Cheméo Relay (1.0)
hfus	19.94	kJ/mol	Joback Method
ie	9.62	eV	Cheméo Relay (1.0)
log10ws	-3.11		Cheméo Relay (1.0)
logp	1.684		Crippen Method
mcvol	122.550	ml/mol	McGowan Method
tb	502.88	K	Cheméo Relay (1.0)
tf	309.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.64	J/mol×K	557.50	Joback Method
cpg	303.82	J/mol×K	592.64	Joback Method
cpg	313.28	J/mol×K	627.78	Joback Method
cpg	322.04	J/mol×K	662.91	Joback Method
cpg	330.13	J/mol×K	698.05	Joback Method
cpg	337.58	J/mol×K	733.19	Joback Method
cpg	344.43	J/mol×K	768.33	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C456713&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

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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