Benzamide, N-(2,5-dimethoxyphenyl)-4-trifluoromethyl-

Inchi: InChI=1S/C16H14F3NO3/c1-22-12-7-8-14(23-2)13(9-12)20-15(21)10-3-5-11(6-4-10)16(1

InchiKey: CPOMMRJDVTZUMI-UHFFFAOYSA-N

Formula: C16H14F3NO3

SMILES: COc1ccc(OC)c(NC(=O)c2ccc(C(F)(F)F)cc2)c1

Mol. weight [g/mol]: 325.28

Physical Properties

Property code	Value	Unit	Source
gf	-551.35	kJ/mol	Joback Method
hf	-855.55	kJ/mol	Joback Method
hfus	35.01	kJ/mol	Joback Method
hvap	72.00	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.975		Crippen Method
mcvol	217.380	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	2221.00		NIST Webbook
rinpol	2221.00		NIST Webbook
tb	777.24	K	Joback Method
tc	992.85	K	Joback Method
tf	511.72	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.69	J/mol×K	777.24	Joback Method
cpg	633.51	J/mol×K	813.17	Joback Method
cpg	645.29	J/mol×K	849.11	Joback Method
cpg	656.07	J/mol×K	885.04	Joback Method
cpg	665.87	J/mol×K	920.98	Joback Method
cpg	674.74	J/mol×K	956.91	Joback Method
cpg	682.72	J/mol×K	992.85	Joback Method

Sources

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=U307251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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