Benzamide, N-(4-methoxyphenyl)-2,3,4-trifluoro-

Inchi: InChI=1S/C14H10F3NO2/c1-20-9-4-2-8(3-5-9)18-14(19)10-6-7-11(15)13(17)12(10)16/h2

InchiKey: LYZBCVKPJODAFH-UHFFFAOYSA-N

Formula: C14H10F3NO2

SMILES: COc1ccc(NC(=O)c2ccc(F)c(F)c2F)cc1

Mol. weight [g/mol]: 281.23

Physical Properties

Property code	Value	Unit	Source
gf	-475.66	kJ/mol	Joback Method
hf	-684.77	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.365		Crippen Method
mcvol	183.330	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	717.27	K	Joback Method
tc	931.23	K	Joback Method
tf	477.05	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.53	J/mol×K	717.27	Joback Method
cpg	497.55	J/mol×K	752.93	Joback Method
cpg	508.70	J/mol×K	788.59	Joback Method
cpg	519.00	J/mol×K	824.25	Joback Method
cpg	528.47	J/mol×K	859.91	Joback Method
cpg	537.13	J/mol×K	895.57	Joback Method
cpg	545.00	J/mol×K	931.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307177&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