Benzamide, N-(4-methoxyphenyl)-4-trifluoromethyl-

Inchi: InChI=1S/C15H12F3NO2/c1-21-13-8-6-12(7-9-13)19-14(20)10-2-4-11(5-3-10)15(16,17)1

InchiKey: XPUFSOPGNYLKJQ-UHFFFAOYSA-N

Formula: C15H12F3NO2

SMILES: COc1ccc(NC(=O)c2ccc(C(F)(F)F)cc2)cc1

Mol. weight [g/mol]: 295.26

Physical Properties

Property code	Value	Unit	Source
gf	-445.14	kJ/mol	Joback Method
hf	-691.22	kJ/mol	Joback Method
hfus	31.62	kJ/mol	Joback Method
hvap	66.70	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.966		Crippen Method
mcvol	197.420	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	726.96	K	Joback Method
tc	946.77	K	Joback Method
tf	465.70	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.86	J/mol×K	726.96	Joback Method
cpg	555.88	J/mol×K	763.59	Joback Method
cpg	567.85	J/mol×K	800.23	Joback Method
cpg	578.82	J/mol×K	836.86	Joback Method
cpg	588.85	J/mol×K	873.50	Joback Method
cpg	598.01	J/mol×K	910.13	Joback Method
cpg	606.36	J/mol×K	946.77	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=U307249&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