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
hf	-786.52	kJ/mol	Cheméo Relay (1.0)
hfus	31.62	kJ/mol	Joback Method
hvap	90.91	kJ/mol	Cheméo Relay (1.0)
ie	8.05	eV	Cheméo Relay (1.0)
log10ws	-4.69		Cheméo Relay (1.0)
logp	3.966		Crippen Method
mcvol	197.420	ml/mol	McGowan Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	636.95	K	Cheméo Relay (1.0)
tf	419.46	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.45100e+01
Coeff. B	1.29822e+00
Coeff. C	-8.60420e-04
Coeff. D	2.03860e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307249&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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