Benzamide, N-(4-bromophenyl)-3-trifluoromethyl-

Inchi: InChI=1S/C14H9BrF3NO/c15-11-4-6-12(7-5-11)19-13(20)9-2-1-3-10(8-9)14(16,17)18/h1

InchiKey: JDUHFWWSDVISOZ-UHFFFAOYSA-N

Formula: C14H9BrF3NO

SMILES: O=C(Nc1ccc(Br)cc1)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 344.13

Physical Properties

Property code	Value	Unit	Source
gf	-334.24	kJ/mol	Joback Method
hf	-512.03	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.720		Crippen Method
mcvol	194.960	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	2201.00		NIST Webbook
tb	747.82	K	Joback Method
tc	984.32	K	Joback Method
tf	492.00	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.39	J/mol×K	747.82	Joback Method
cpg	510.58	J/mol×K	787.24	Joback Method
cpg	520.76	J/mol×K	826.65	Joback Method
cpg	530.03	J/mol×K	866.07	Joback Method
cpg	538.49	J/mol×K	905.49	Joback Method
cpg	546.26	J/mol×K	944.90	Joback Method
cpg	553.42	J/mol×K	984.32	Joback Method

Sources

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=U306938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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