N-(4-Bromophenyl)-2,3,4,5,6-pentafluorobenzamid

Other names: Benzamide, N-(4-bromophenyl)-2,3,4,5,6-pentafluoro-
Inchi: InChI=1S/C13H5BrF5NO/c14-5-1-3-6(4-2-5)20-13(21)7-8(15)10(17)12(19)11(18)9(7)16/h
InchiKey: IDWYRSRIRSQVBS-UHFFFAOYSA-N
Formula: C13H5BrF5NO
SMILES: O=C(Nc1ccc(Br)cc1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 366.08
CAS: 63462-61-3

Physical Properties

Property code	Value	Unit	Source
gf	-773.64	kJ/mol	Joback Method
hf	-920.74	kJ/mol	Joback Method
hfus	42.56	kJ/mol	Joback Method
hvap	68.59	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	4.397		Crippen Method
mcvol	184.410	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	746.63	K	Joback Method
tc	960.66	K	Joback Method
tf	529.57	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.49	J/mol×K	746.63	Joback Method
cpg	463.57	J/mol×K	782.30	Joback Method
cpg	471.95	J/mol×K	817.97	Joback Method
cpg	479.67	J/mol×K	853.65	Joback Method
cpg	486.76	J/mol×K	889.32	Joback Method
cpg	493.25	J/mol×K	924.99	Joback Method

cpg	499.16	J/mol×K	960.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63462613&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