N-(4-Bromo-phenyl)-4-ethyl-benzamide

Other names: Benzamide, N-(4-bromophenyl)-4-ethyl-
Inchi: InChI=1S/C15H14BrNO/c1-2-11-3-5-12(6-4-11)15(18)17-14-9-7-13(16)8-10-14/h3-10H,2
InchiKey: AIQFMLWABGCAHE-UHFFFAOYSA-N
Formula: C15H14BrNO
SMILES: CCc1ccc(C(=O)Nc2ccc(Br)cc2)cc1
Mol. weight [g/mol]: 304.18
CAS: 300670-74-0

Physical Properties

Property code	Value	Unit	Source
gf	255.77	kJ/mol	Joback Method
hf	64.41	kJ/mol	Joback Method
hfus	33.89	kJ/mol	Joback Method
hvap	74.48	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.264		Crippen Method
mcvol	203.740	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	2509.00		NIST Webbook
tb	776.12	K	Joback Method
tc	1026.15	K	Joback Method
tf	499.08	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.91	J/mol×K	776.12	Joback Method
cpg	539.14	J/mol×K	817.79	Joback Method
cpg	551.25	J/mol×K	859.46	Joback Method
cpg	562.33	J/mol×K	901.14	Joback Method
cpg	572.48	J/mol×K	942.81	Joback Method
cpg	581.78	J/mol×K	984.48	Joback Method
cpg	590.31	J/mol×K	1026.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C300670740&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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