Benzamide, N-(4-bromophenyl)-4-butyl-

Inchi: InChI=1S/C17H18BrNO/c1-2-3-4-13-5-7-14(8-6-13)17(20)19-16-11-9-15(18)10-12-16/h5
InchiKey: GGCPPTSCKWIRBQ-UHFFFAOYSA-N
Formula: C17H18BrNO
SMILES: CCCCc1ccc(C(=O)Nc2ccc(Br)cc2)cc1
Mol. weight [g/mol]: 332.24

Physical Properties

Property code	Value	Unit	Source
gf	272.61	kJ/mol	Joback Method
hf	23.13	kJ/mol	Joback Method
hfus	39.07	kJ/mol	Joback Method
hvap	78.93	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.044		Crippen Method
mcvol	231.920	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	2743.00		NIST Webbook
tb	821.88	K	Joback Method
tc	1062.55	K	Joback Method
tf	521.62	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.43	J/mol×K	821.88	Joback Method
cpg	648.31	J/mol×K	861.99	Joback Method
cpg	661.09	J/mol×K	902.10	Joback Method
cpg	672.86	J/mol×K	942.21	Joback Method
cpg	683.71	J/mol×K	982.32	Joback Method
cpg	693.73	J/mol×K	1022.43	Joback Method
cpg	703.00	J/mol×K	1062.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306994&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