Propanamide, N-(4-bromophenyl)-3-phenyl-

Inchi: InChI=1S/C15H14BrNO/c16-13-7-9-14(10-8-13)17-15(18)11-6-12-4-2-1-3-5-12/h1-5,7-10
InchiKey: HGPWLPIFXDCULJ-UHFFFAOYSA-N
Formula: C15H14BrNO
SMILES: O=C(CCc1ccccc1)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 304.18

Physical Properties

Property code	Value	Unit	Source
gf	265.40	kJ/mol	Joback Method
hf	75.88	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	73.81	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.020		Crippen Method
mcvol	203.740	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	2423.00		NIST Webbook
rinpol	2423.00		NIST Webbook
tb	771.14	K	Joback Method
tc	1020.43	K	Joback Method
tf	486.56	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.37	J/mol×K	771.14	Joback Method
cpg	540.71	J/mol×K	812.69	Joback Method
cpg	552.90	J/mol×K	854.24	Joback Method
cpg	564.05	J/mol×K	895.79	Joback Method
cpg	574.26	J/mol×K	937.34	Joback Method
cpg	583.62	J/mol×K	978.88	Joback Method
cpg	592.23	J/mol×K	1020.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308118&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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