Benzamide, N-(1-naphthyl)-3-bromo-

Inchi: InChI=1S/C17H12BrNO/c18-14-8-3-7-13(11-14)17(20)19-16-10-4-6-12-5-1-2-9-15(12)16
InchiKey: XKNZEZOUWZIZTR-UHFFFAOYSA-N
Formula: C17H12BrNO
SMILES: O=C(Nc1cccc2ccccc12)c1cccc(Br)c1
Mol. weight [g/mol]: 326.19

Physical Properties

Property code	Value	Unit	Source
gf	379.26	kJ/mol	Joback Method
hf	214.20	kJ/mol	Joback Method
hfus	36.09	kJ/mol	Joback Method
hvap	80.57	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	4.855		Crippen Method
mcvol	212.460	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	2758.00		NIST Webbook
tb	840.86	K	Joback Method
tc	1107.55	K	Joback Method
tf	554.32	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.12	J/mol×K	840.86	Joback Method
cpg	570.25	J/mol×K	885.31	Joback Method
cpg	581.40	J/mol×K	929.76	Joback Method
cpg	591.75	J/mol×K	974.21	Joback Method
cpg	601.44	J/mol×K	1018.65	Joback Method
cpg	610.65	J/mol×K	1063.10	Joback Method
cpg	619.53	J/mol×K	1107.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307160&Units=SI

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