Propanamide, N-(1-naphthyl)-2-bromo-

Inchi: InChI=1S/C13H12BrNO/c1-9(14)13(16)15-12-8-4-6-10-5-2-3-7-11(10)12/h2-9H,1H3,(H,1
InchiKey: DWJREIMLLUYESG-UHFFFAOYSA-N
Formula: C13H12BrNO
SMILES: CC(Br)C(=O)Nc1cccc2ccccc12
Mol. weight [g/mol]: 278.14

Physical Properties

Property code	Value	Unit	Source
gf	240.36	kJ/mol	Joback Method
hf	66.42	kJ/mol	Joback Method
hfus	28.56	kJ/mol	Joback Method
hvap	68.34	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.562		Crippen Method
mcvol	179.860	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook
tb	717.24	K	Joback Method
tc	964.79	K	Joback Method
tf	455.30	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.30	J/mol×K	717.24	Joback Method
cpg	456.79	J/mol×K	758.50	Joback Method
cpg	468.26	J/mol×K	799.76	Joback Method
cpg	478.84	J/mol×K	841.01	Joback Method
cpg	488.63	J/mol×K	882.27	Joback Method
cpg	497.73	J/mol×K	923.53	Joback Method
cpg	506.26	J/mol×K	964.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307480&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