Benzamide, 2-bromo-N-hexyl-

Inchi: InChI=1S/C13H18BrNO/c1-2-3-4-7-10-15-13(16)11-8-5-6-9-12(11)14/h5-6,8-9H,2-4,7,10
InchiKey: IPMUKUSNHMTNKR-UHFFFAOYSA-N
Formula: C13H18BrNO
SMILES: CCCCCCNC(=O)c1ccccc1Br
Mol. weight [g/mol]: 284.19

Physical Properties

Property code	Value	Unit	Source
gf	136.15	kJ/mol	Joback Method
hf	-119.37	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.759		Crippen Method
mcvol	199.320	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	2115.00		NIST Webbook
rinpol	2115.00		NIST Webbook
tb	698.70	K	Joback Method
tc	915.58	K	Joback Method
tf	437.60	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.74	J/mol×K	698.70	Joback Method
cpg	524.84	J/mol×K	734.85	Joback Method
cpg	538.03	J/mol×K	770.99	Joback Method
cpg	550.34	J/mol×K	807.14	Joback Method
cpg	561.84	J/mol×K	843.29	Joback Method
cpg	572.56	J/mol×K	879.43	Joback Method
cpg	582.57	J/mol×K	915.58	Joback Method

Sources

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=U407118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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