Benzamide, 2-bromo-N-ethyl-N-hexadecyl-

Inchi: InChI=1S/C25H42BrNO/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-19-22-27(4-2)25(28)23-20
InchiKey: JYQQCXBXQBQSIN-UHFFFAOYSA-N
Formula: C25H42BrNO
SMILES: CCCCCCCCCCCCCCCCN(CC)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 452.51

Physical Properties

Property code	Value	Unit	Source
gf	258.58	kJ/mol	Joback Method
hf	-352.99	kJ/mol	Joback Method
hfus	64.06	kJ/mol	Joback Method
hvap	89.41	kJ/mol	Joback Method
log10ws	-9.48		Crippen Method
logp	8.393		Crippen Method
mcvol	368.400	ml/mol	McGowan Method
pc	993.88	kPa	Joback Method
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
tb	935.53	K	Joback Method
tc	1146.05	K	Joback Method
tf	552.65	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.15	J/mol×K	935.53	Joback Method
cpg	1208.85	J/mol×K	970.62	Joback Method
cpg	1226.44	J/mol×K	1005.70	Joback Method
cpg	1243.02	J/mol×K	1040.79	Joback Method
cpg	1258.68	J/mol×K	1075.88	Joback Method
cpg	1273.51	J/mol×K	1110.96	Joback Method
cpg	1287.59	J/mol×K	1146.05	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=U415369&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

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