Benzamide, 3-bromo-N-(2-ethylhexyl)-

Inchi: InChI=1S/C15H22BrNO/c1-3-5-7-12(4-2)11-17-15(18)13-8-6-9-14(16)10-13/h6,8-10,12H
InchiKey: IYEAXBBMYLCASU-UHFFFAOYSA-N
Formula: C15H22BrNO
SMILES: CCCCC(CC)CNC(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 312.25

Physical Properties

Property code	Value	Unit	Source
gf	150.55	kJ/mol	Joback Method
hf	-165.93	kJ/mol	Joback Method
hfus	36.72	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.395		Crippen Method
mcvol	227.500	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	2263.00		NIST Webbook
rinpol	2263.00		NIST Webbook
tb	744.02	K	Joback Method
tc	958.39	K	Joback Method
tf	445.14	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.14	J/mol×K	744.02	Joback Method
cpg	633.31	J/mol×K	779.75	Joback Method
cpg	647.49	J/mol×K	815.48	Joback Method
cpg	660.74	J/mol×K	851.20	Joback Method
cpg	673.11	J/mol×K	886.93	Joback Method
cpg	684.67	J/mol×K	922.66	Joback Method
cpg	695.46	J/mol×K	958.39	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=U407209&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