Benzamide, 2-bromo-N-ethyl-N-2-ethylhexyl-

Inchi: InChI=1S/C17H26BrNO/c1-4-7-10-14(5-2)13-19(6-3)17(20)15-11-8-9-12-16(15)18/h8-9,1
InchiKey: ONNNJHKMWSCUBD-UHFFFAOYSA-N
Formula: C17H26BrNO
SMILES: CCCCC(CC)CN(CC)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 340.30

Physical Properties

Property code	Value	Unit	Source
gf	188.78	kJ/mol	Joback Method
hf	-193.15	kJ/mol	Joback Method
hfus	39.82	kJ/mol	Joback Method
hvap	71.21	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.128		Crippen Method
mcvol	255.680	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	2309.00		NIST Webbook
rinpol	2309.00		NIST Webbook
tb	752.05	K	Joback Method
tc	959.10	K	Joback Method
tf	447.49	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.95	J/mol×K	752.05	Joback Method
cpg	729.53	J/mol×K	786.56	Joback Method
cpg	745.08	J/mol×K	821.07	Joback Method
cpg	759.65	J/mol×K	855.58	Joback Method
cpg	773.31	J/mol×K	890.09	Joback Method
cpg	786.12	J/mol×K	924.59	Joback Method
cpg	798.15	J/mol×K	959.10	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=U415361&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