Benzamide, 4-bromo-N-ethyl-N-3-methylbutyl-

Inchi: InChI=1S/C14H20BrNO/c1-4-16(10-9-11(2)3)14(17)12-5-7-13(15)8-6-12/h5-8,11H,4,9-10
InchiKey: PXXZYNDKZFEMHR-UHFFFAOYSA-N
Formula: C14H20BrNO
SMILES: CCN(CCC(C)C)C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 298.22

Physical Properties

Property code	Value	Unit	Source
gf	163.52	kJ/mol	Joback Method
hf	-131.23	kJ/mol	Joback Method
hfus	32.05	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.957		Crippen Method
mcvol	213.410	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	683.41	K	Joback Method
tc	898.75	K	Joback Method
tf	413.68	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.42	J/mol×K	683.41	Joback Method
cpg	565.08	J/mol×K	719.30	Joback Method
cpg	579.70	J/mol×K	755.19	Joback Method
cpg	593.35	J/mol×K	791.08	Joback Method
cpg	606.10	J/mol×K	826.97	Joback Method
cpg	617.99	J/mol×K	862.86	Joback Method
cpg	629.09	J/mol×K	898.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415453&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

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