Benzamide, 4-butyl-N-butyl-N-isobutyl-

Inchi: InChI=1S/C19H31NO/c1-5-7-9-17-10-12-18(13-11-17)19(21)20(14-8-6-2)15-16(3)4/h10-1
InchiKey: PDFVTUBWXFDHNH-UHFFFAOYSA-N
Formula: C19H31NO
SMILES: CCCCc1ccc(C(=O)N(CCCC)CC(C)C)cc1
Mol. weight [g/mol]: 289.46

Physical Properties

Property code	Value	Unit	Source
gf	191.30	kJ/mol	Joback Method
hf	-260.76	kJ/mol	Joback Method
hfus	39.71	kJ/mol	Joback Method
hvap	69.23	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.928		Crippen Method
mcvol	266.360	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2694.00		NIST Webbook
rinpol	2694.00		NIST Webbook
tb	731.65	K	Joback Method
tc	925.14	K	Joback Method
tf	410.23	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.65	J/mol×K	731.65	Joback Method
cpg	798.31	J/mol×K	763.90	Joback Method
cpg	815.91	J/mol×K	796.15	Joback Method
cpg	832.49	J/mol×K	828.40	Joback Method
cpg	848.09	J/mol×K	860.64	Joback Method
cpg	862.78	J/mol×K	892.89	Joback Method
cpg	876.60	J/mol×K	925.14	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=U415872&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