Benzamide, 4-butyl-N-butyl-N-3-methylbutyl-

Inchi: InChI=1S/C20H33NO/c1-5-7-9-18-10-12-19(13-11-18)20(22)21(15-8-6-2)16-14-17(3)4/h1
InchiKey: MKZIWULMBBKIDB-UHFFFAOYSA-N
Formula: C20H33NO
SMILES: CCCCc1ccc(C(=O)N(CCCC)CCC(C)C)cc1
Mol. weight [g/mol]: 303.48

Physical Properties

Property code	Value	Unit	Source
gf	199.72	kJ/mol	Joback Method
hf	-281.40	kJ/mol	Joback Method
hfus	42.30	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.318		Crippen Method
mcvol	280.450	ml/mol	McGowan Method
pc	1319.43	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	754.53	K	Joback Method
tc	947.21	K	Joback Method
tf	421.50	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.92	J/mol×K	754.53	Joback Method
cpg	856.78	J/mol×K	786.64	Joback Method
cpg	874.57	J/mol×K	818.76	Joback Method
cpg	891.33	J/mol×K	850.87	Joback Method
cpg	907.12	J/mol×K	882.98	Joback Method
cpg	921.97	J/mol×K	915.09	Joback Method
cpg	935.95	J/mol×K	947.21	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=U415874&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