Benzamide, 2-methyl-N-butyl-N-3-methylbutyl-

Inchi: InChI=1S/C17H27NO/c1-5-6-12-18(13-11-14(2)3)17(19)16-10-8-7-9-15(16)4/h7-10,14H,
InchiKey: URWRZXPOGMMIPW-UHFFFAOYSA-N
Formula: C17H27NO
SMILES: CCCCN(CCC(C)C)C(=O)c1ccccc1C
Mol. weight [g/mol]: 261.40

Physical Properties

Property code	Value	Unit	Source
gf	174.46	kJ/mol	Joback Method
hf	-219.48	kJ/mol	Joback Method
hfus	34.53	kJ/mol	Joback Method
hvap	64.78	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.283		Crippen Method
mcvol	238.180	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook
tb	685.89	K	Joback Method
tc	882.46	K	Joback Method
tf	387.69	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.24	J/mol×K	685.89	Joback Method
cpg	684.45	J/mol×K	718.65	Joback Method
cpg	701.60	J/mol×K	751.41	Joback Method
cpg	717.75	J/mol×K	784.18	Joback Method
cpg	732.95	J/mol×K	816.94	Joback Method
cpg	747.23	J/mol×K	849.70	Joback Method
cpg	760.65	J/mol×K	882.46	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=U415731&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