Benzamide, 2-methyl-N-butyl-N-isobutyl-

Inchi: InChI=1S/C16H25NO/c1-5-6-11-17(12-13(2)3)16(18)15-10-8-7-9-14(15)4/h7-10,13H,5-6
InchiKey: NZLRCQDTARKGRB-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CCCCN(CC(C)C)C(=O)c1ccccc1C
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
gf	166.04	kJ/mol	Joback Method
hf	-198.84	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	62.55	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.893		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	663.01	K	Joback Method
tc	861.76	K	Joback Method
tf	376.42	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.25	J/mol×K	663.01	Joback Method
cpg	629.17	J/mol×K	696.13	Joback Method
cpg	646.06	J/mol×K	729.26	Joback Method
cpg	661.95	J/mol×K	762.38	Joback Method
cpg	676.88	J/mol×K	795.51	Joback Method
cpg	690.92	J/mol×K	828.63	Joback Method
cpg	704.09	J/mol×K	861.76	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=U415729&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