Benzamide, 4-butyl-N-isobutyl-

Inchi: InChI=1S/C15H23NO/c1-4-5-6-13-7-9-14(10-8-13)15(17)16-11-12(2)3/h7-10,12H,4-6,11
InchiKey: JUVNNJASLWYUQA-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CCCCc1ccc(C(=O)NCC(C)C)cc1
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
gf	136.23	kJ/mol	Joback Method
hf	-192.26	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.415		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	677.86	K	Joback Method
tc	881.81	K	Joback Method
tf	385.34	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.38	J/mol×K	677.86	Joback Method
cpg	592.11	J/mol×K	711.85	Joback Method
cpg	607.84	J/mol×K	745.84	Joback Method
cpg	622.63	J/mol×K	779.84	Joback Method
cpg	636.50	J/mol×K	813.83	Joback Method
cpg	649.50	J/mol×K	847.82	Joback Method
cpg	661.67	J/mol×K	881.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407447&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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