Benzamide, n,n-dibutyl-

Other names: Di-N-n-butylbenzoic acid amide
N,N-Dibutylbenzamide
Inchi: InChI=1S/C15H23NO/c1-3-5-12-16(13-6-4-2)15(17)14-10-8-7-9-11-14/h7-11H,3-6,12-13
InchiKey: RYGJQVQEGCQNHM-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CCCCN(CCCC)C(=O)c1ccccc1
Mol. weight [g/mol]: 233.36

Physical Properties

Property code	Value	Unit	Source
af	0.6875		Cheméo Relay (1.0)
gf	169.69	kJ/mol	Joback Method
hf	-217.88	kJ/mol	Cheméo Relay (1.0)
hfus	33.27	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Cheméo Relay (1.0)
ie	8.29	eV	Cheméo Relay (1.0)
log10ws	-3.93		Cheméo Relay (1.0)
logp	3.729		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	593.02	K	Cheméo Relay (1.0)
tc	786.05	K	Cheméo Relay (1.0)
tf	270.02	K	Cheméo Relay (1.0)
vc	0.775	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.20	J/mol×K	635.59	Joback Method
cpg	574.64	J/mol×K	668.39	Joback Method
cpg	591.06	J/mol×K	701.19	Joback Method
cpg	606.51	J/mol×K	733.98	Joback Method

cpg	621.04	J/mol×K	766.78	Joback Method
cpg	634.68	J/mol×K	799.58	Joback Method
cpg	647.49	J/mol×K	832.38	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25033652&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
ie: Ionization energy
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