Benzamide, 4-butyl-N-butyl-N-propyl-

Inchi: InChI=1S/C18H29NO/c1-4-7-9-16-10-12-17(13-11-16)18(20)19(14-6-3)15-8-5-2/h10-13H
InchiKey: RWMIIPKKGDJDAP-UHFFFAOYSA-N
Formula: C18H29NO
SMILES: CCCCc1ccc(C(=O)N(CCC)CCCC)cc1
Mol. weight [g/mol]: 275.43

Physical Properties

Property code	Value	Unit	Source
gf	185.32	kJ/mol	Joback Method
hf	-234.84	kJ/mol	Joback Method
hfus	40.65	kJ/mol	Joback Method
hvap	67.39	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.682		Crippen Method
mcvol	252.270	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook
tb	709.21	K	Joback Method
tc	901.18	K	Joback Method
tf	413.96	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.93	J/mol×K	709.21	Joback Method
cpg	740.08	J/mol×K	741.20	Joback Method
cpg	757.22	J/mol×K	773.20	Joback Method
cpg	773.38	J/mol×K	805.19	Joback Method
cpg	788.62	J/mol×K	837.19	Joback Method
cpg	802.97	J/mol×K	869.18	Joback Method
cpg	816.49	J/mol×K	901.18	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=U415871&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