Benzamide, 4-butyl-N-butyl-N-hept-2-yl-

Inchi: InChI=1S/C22H37NO/c1-5-8-11-12-19(4)23(18-10-7-3)22(24)21-16-14-20(15-17-21)13-9
InchiKey: BIYAFVJKBBNWGF-UHFFFAOYSA-N
Formula: C22H37NO
SMILES: CCCCCC(C)N(CCCC)C(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 331.54

Physical Properties

Property code	Value	Unit	Source
gf	216.56	kJ/mol	Joback Method
hf	-322.68	kJ/mol	Joback Method
hfus	47.48	kJ/mol	Joback Method
hvap	75.91	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.240		Crippen Method
mcvol	308.630	ml/mol	McGowan Method
pc	1153.00	kPa	Joback Method
rinpol	2983.00		NIST Webbook
rinpol	2983.00		NIST Webbook
tb	800.29	K	Joback Method
tc	993.03	K	Joback Method
tf	444.04	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.23	J/mol×K	800.29	Joback Method
cpg	976.50	J/mol×K	832.41	Joback Method
cpg	994.67	J/mol×K	864.54	Joback Method
cpg	1011.79	J/mol×K	896.66	Joback Method
cpg	1027.90	J/mol×K	928.78	Joback Method
cpg	1043.08	J/mol×K	960.91	Joback Method
cpg	1057.36	J/mol×K	993.03	Joback Method

Sources

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=U415876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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