Benzamide, 4-butyl-N-decyl-

Inchi: InChI=1S/C21H35NO/c1-3-5-7-8-9-10-11-12-18-22-21(23)20-16-14-19(15-17-20)13-6-4-
InchiKey: KHBHMUGFJFNUFE-UHFFFAOYSA-N
Formula: C21H35NO
SMILES: CCCCCCCCCCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 317.51

Physical Properties

Property code	Value	Unit	Source
gf	189.19	kJ/mol	Joback Method
hf	-310.82	kJ/mol	Joback Method
hfus	50.50	kJ/mol	Joback Method
hvap	78.46	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.900		Crippen Method
mcvol	294.540	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	2725.00		NIST Webbook
rinpol	2725.00		NIST Webbook
tb	815.58	K	Joback Method
tc	1010.53	K	Joback Method
tf	467.96	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.49	J/mol×K	815.58	Joback Method
cpg	935.60	J/mol×K	848.07	Joback Method
cpg	952.66	J/mol×K	880.56	Joback Method
cpg	968.71	J/mol×K	913.05	Joback Method
cpg	983.80	J/mol×K	945.54	Joback Method
cpg	997.98	J/mol×K	978.04	Joback Method
cpg	1011.31	J/mol×K	1010.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407457&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

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