Benzamide, 4-ethyl-N-butyl-N-2-ethylhexyl-

Inchi: InChI=1S/C21H35NO/c1-5-9-11-19(8-4)17-22(16-10-6-2)21(23)20-14-12-18(7-3)13-15-2(
InchiKey: YGEZUWMXCWXCED-UHFFFAOYSA-N
Formula: C21H35NO
SMILES: CCCCC(CC)CN(CCCC)C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 317.51

Physical Properties

Property code	Value	Unit	Source
gf	208.14	kJ/mol	Joback Method
hf	-302.04	kJ/mol	Joback Method
hfus	44.89	kJ/mol	Joback Method
hvap	73.68	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.708		Crippen Method
mcvol	294.540	ml/mol	McGowan Method
pc	1232.01	kPa	Joback Method
rinpol	2993.00		NIST Webbook
rinpol	2993.00		NIST Webbook
tb	777.41	K	Joback Method
tc	969.82	K	Joback Method
tf	432.77	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.13	J/mol×K	777.41	Joback Method
cpg	916.20	J/mol×K	809.48	Joback Method
cpg	934.17	J/mol×K	841.55	Joback Method
cpg	951.11	J/mol×K	873.61	Joback Method
cpg	967.06	J/mol×K	905.68	Joback Method
cpg	982.08	J/mol×K	937.75	Joback Method
cpg	996.21	J/mol×K	969.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415894&Units=SI

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