Benzamide, N,N-bis(2-ethylhexyl)-4-butyl-

Inchi: InChI=1S/C27H47NO/c1-6-11-14-23(9-4)21-28(22-24(10-5)15-12-7-2)27(29)26-19-17-25
InchiKey: UZXKSCLIHROMHE-UHFFFAOYSA-N
Formula: C27H47NO
SMILES: CCCCc1ccc(C(=O)N(CC(CC)CCCC)CC(CC)CCCC)cc1
Mol. weight [g/mol]: 401.67

Physical Properties

Property code	Value	Unit	Source
gf	256.22	kJ/mol	Joback Method
hf	-431.16	kJ/mol	Joback Method
hfus	56.91	kJ/mol	Joback Method
hvap	86.65	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	7.904		Crippen Method
mcvol	379.080	ml/mol	McGowan Method
pc	856.47	kPa	Joback Method
rinpol	2707.00		NIST Webbook
tb	914.25	K	Joback Method
tc	1119.70	K	Joback Method
tf	485.39	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.24	J/mol×K	914.25	Joback Method
cpg	1290.01	J/mol×K	948.49	Joback Method
cpg	1309.48	J/mol×K	982.73	Joback Method
cpg	1327.76	J/mol×K	1016.98	Joback Method
cpg	1344.91	J/mol×K	1051.22	Joback Method
cpg	1361.03	J/mol×K	1085.46	Joback Method
cpg	1376.18	J/mol×K	1119.70	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=U308570&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