Benzamide, N,N-dinonyl-4-ethyl-

Inchi: InChI=1S/C27H47NO/c1-4-7-9-11-13-15-17-23-28(24-18-16-14-12-10-8-5-2)27(29)26-21
InchiKey: IOOSLTGCIUSZMN-UHFFFAOYSA-N
Formula: C27H47NO
SMILES: CCCCCCCCCN(CCCCCCCCC)C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 401.67

Physical Properties

Property code	Value	Unit	Source
gf	261.10	kJ/mol	Joback Method
hf	-420.60	kJ/mol	Joback Method
hfus	63.96	kJ/mol	Joback Method
hvap	87.42	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.192		Crippen Method
mcvol	379.080	ml/mol	McGowan Method
pc	848.50	kPa	Joback Method
rinpol	2989.00		NIST Webbook
rinpol	2989.00		NIST Webbook
tb	915.13	K	Joback Method
tc	1120.39	K	Joback Method
tf	515.39	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.45	J/mol×K	915.13	Joback Method
cpg	1289.25	J/mol×K	949.34	Joback Method
cpg	1308.79	J/mol×K	983.55	Joback Method
cpg	1327.16	J/mol×K	1017.76	Joback Method
cpg	1344.43	J/mol×K	1051.97	Joback Method
cpg	1360.69	J/mol×K	1086.18	Joback Method
cpg	1376.01	J/mol×K	1120.39	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=U308551&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