Benzamide, 4-butyl-N-hexadecyl-

Inchi: InChI=1S/C27H47NO/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-24-28-27(29)26-22-20-2
InchiKey: LSEBGNRMCWRFBQ-UHFFFAOYSA-N
Formula: C27H47NO
SMILES: CCCCCCCCCCCCCCCCCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 401.67

Physical Properties

Property code	Value	Unit	Source
gf	239.71	kJ/mol	Joback Method
hf	-434.66	kJ/mol	Joback Method
hfus	66.04	kJ/mol	Joback Method
hvap	91.82	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	8.240		Crippen Method
mcvol	379.080	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	3358.00		NIST Webbook
rinpol	3358.00		NIST Webbook
tb	952.86	K	Joback Method
tc	1166.88	K	Joback Method
tf	535.58	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1290.16	J/mol×K	952.86	Joback Method
cpg	1310.40	J/mol×K	988.53	Joback Method
cpg	1329.33	J/mol×K	1024.20	Joback Method
cpg	1347.04	J/mol×K	1059.87	Joback Method
cpg	1363.62	J/mol×K	1095.54	Joback Method
cpg	1379.14	J/mol×K	1131.21	Joback Method
cpg	1393.70	J/mol×K	1166.88	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=U407460&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