Benzamide, 4-butyl-N-dodecyl-

Inchi: InChI=1S/C23H39NO/c1-3-5-7-8-9-10-11-12-13-14-20-24-23(25)22-18-16-21(17-19-22)1
InchiKey: IBBILQMGVQQKQK-UHFFFAOYSA-N
Formula: C23H39NO
SMILES: CCCCCCCCCCCCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 345.56

Physical Properties

Property code	Value	Unit	Source
gf	206.03	kJ/mol	Joback Method
hf	-352.10	kJ/mol	Joback Method
hfus	55.68	kJ/mol	Joback Method
hvap	82.91	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	6.680		Crippen Method
mcvol	322.720	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	2942.00		NIST Webbook
rinpol	2942.00		NIST Webbook
tb	861.34	K	Joback Method
tc	1059.32	K	Joback Method
tf	490.50	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.02	J/mol×K	861.34	Joback Method
cpg	1057.69	J/mol×K	894.34	Joback Method
cpg	1075.25	J/mol×K	927.33	Joback Method
cpg	1091.75	J/mol×K	960.33	Joback Method
cpg	1107.24	J/mol×K	993.32	Joback Method
cpg	1121.80	J/mol×K	1026.32	Joback Method
cpg	1135.47	J/mol×K	1059.32	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=U407458&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