Benzamide, N,N-didecyl-4-butyl-

Inchi: InChI=1S/C31H55NO/c1-4-7-10-12-14-16-18-20-27-32(28-21-19-17-15-13-11-8-5-2)31(3
InchiKey: KCPZMQXUCJUWGY-UHFFFAOYSA-N
Formula: C31H55NO
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 457.77

Physical Properties

Property code	Value	Unit	Source
gf	294.78	kJ/mol	Joback Method
hf	-503.16	kJ/mol	Joback Method
hfus	74.32	kJ/mol	Joback Method
hvap	96.33	kJ/mol	Joback Method
log10ws	-10.79		Crippen Method
logp	9.753		Crippen Method
mcvol	435.440	ml/mol	McGowan Method
pc	686.37	kPa	Joback Method
rinpol	3700.00		NIST Webbook
rinpol	3700.00		NIST Webbook
tb	1006.65	K	Joback Method
tc	1240.52	K	Joback Method
tf	560.47	K	Joback Method
vc	1.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1528.26	J/mol×K	1006.65	Joback Method
cpg	1551.52	J/mol×K	1045.63	Joback Method
cpg	1573.23	J/mol×K	1084.61	Joback Method
cpg	1593.54	J/mol×K	1123.58	Joback Method
cpg	1612.58	J/mol×K	1162.56	Joback Method
cpg	1630.49	J/mol×K	1201.54	Joback Method
cpg	1647.40	J/mol×K	1240.52	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=U308575&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