Benzamide, 4-methyl-N-butyl-N-nonyl-

Inchi: InChI=1S/C21H35NO/c1-4-6-8-9-10-11-12-18-22(17-7-5-2)21(23)20-15-13-19(3)14-16-2
InchiKey: MFCNZXYFKOPCTJ-UHFFFAOYSA-N
Formula: C21H35NO
SMILES: CCCCCCCCCN(CCCC)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 317.51

Physical Properties

Property code	Value	Unit	Source
gf	210.58	kJ/mol	Joback Method
hf	-296.76	kJ/mol	Joback Method
hfus	48.42	kJ/mol	Joback Method
hvap	74.07	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.988		Crippen Method
mcvol	294.540	ml/mol	McGowan Method
pc	1225.12	kPa	Joback Method
rinpol	3150.00		NIST Webbook
tb	777.85	K	Joback Method
tc	968.26	K	Joback Method
tf	447.77	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.65	J/mol×K	777.85	Joback Method
cpg	915.51	J/mol×K	809.58	Joback Method
cpg	933.31	J/mol×K	841.32	Joback Method
cpg	950.11	J/mol×K	873.05	Joback Method
cpg	965.94	J/mol×K	904.79	Joback Method
cpg	980.87	J/mol×K	936.52	Joback Method
cpg	994.95	J/mol×K	968.26	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=U415927&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