Benzamide, N,N-diheptyl-4-methyl-

Inchi: InChI=1S/C22H37NO/c1-4-6-8-10-12-18-23(19-13-11-9-7-5-2)22(24)21-16-14-20(3)15-1
InchiKey: TWRFQRPCDUFJKS-UHFFFAOYSA-N
Formula: C22H37NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 331.54

Physical Properties

Property code	Value	Unit	Source
gf	219.00	kJ/mol	Joback Method
hf	-317.40	kJ/mol	Joback Method
hfus	51.01	kJ/mol	Joback Method
hvap	76.29	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.378		Crippen Method
mcvol	308.630	ml/mol	McGowan Method
pc	1146.76	kPa	Joback Method
rinpol	2466.00		NIST Webbook
rinpol	2466.00		NIST Webbook
tb	800.73	K	Joback Method
tc	991.77	K	Joback Method
tf	459.04	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.75	J/mol×K	800.73	Joback Method
cpg	975.85	J/mol×K	832.57	Joback Method
cpg	993.88	J/mol×K	864.41	Joback Method
cpg	1010.88	J/mol×K	896.25	Joback Method
cpg	1026.91	J/mol×K	928.09	Joback Method
cpg	1042.02	J/mol×K	959.93	Joback Method
cpg	1056.26	J/mol×K	991.77	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=U308465&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

Latest version available from:

https://www.chemeo.com/cid/84-516-6/Benzamide-N-N-diheptyl-4-methyl.pdf

Generated by Cheméo on 2024-10-12 02:11:21.878140656 +0000 UTC m=+3279944.515109904.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.