

Benzamide, 4-butyl-N-butyl-N-heptyl-

Inchi:	InChI=1S/C22H37NO/c1-4-7-10-11-12-19-23(18-9-6-3)22(24)21-16-14-20(15-17-21)13-8
InchiKey:	CWIRWBLFLVTDZ-UHFFFAOYSA-N
Formula:	C22H37NO
SMILES:	CCCCCCN(CCCC)C(=O)c1ccc(CCCC)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	-7.02		Crippen Method
logp	6.242		Crippen Method
mvol	308.630	ml/mol	McGowan Method
pc	1146.76	kPa	Joback Method
rinpol	3139.00		NIST Webbook
rinpol	3139.00		NIST Webbook
tb	800.73	K	Joback Method
tc	991.77	K	Joback Method
tf	459.04	K	Joback Method
vc	1.183	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415879&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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