Benzamide, N,N-diheptyl-4-butyl-

Inchi: InChI=1S/C25H43NO/c1-4-7-10-12-14-21-26(22-15-13-11-8-5-2)25(27)24-19-17-23(18-2
InchiKey: BJPXLJONQWMDGI-UHFFFAOYSA-N
Formula: C25H43NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 373.62

Physical Properties

Property code	Value	Unit	Source
gf	244.26	kJ/mol	Joback Method
hf	-379.32	kJ/mol	Joback Method
hfus	58.78	kJ/mol	Joback Method
hvap	82.97	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.412		Crippen Method
mcvol	350.900	ml/mol	McGowan Method
pc	952.01	kPa	Joback Method
rinpol	2751.00		NIST Webbook
tb	869.37	K	Joback Method
tc	1066.48	K	Joback Method
tf	492.85	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1141.75	J/mol×K	869.37	Joback Method
cpg	1161.74	J/mol×K	902.22	Joback Method
cpg	1180.56	J/mol×K	935.07	Joback Method
cpg	1198.28	J/mol×K	967.93	Joback Method
cpg	1214.97	J/mol×K	1000.78	Joback Method
cpg	1230.69	J/mol×K	1033.63	Joback Method
cpg	1245.51	J/mol×K	1066.48	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=U308571&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

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