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

Inchi: InChI=1S/C26H45NO/c1-4-7-10-12-14-16-23-27(22-15-13-11-8-5-2)26(28)25-20-18-24(1
InchiKey: FWQXKOBGUZUFKT-UHFFFAOYSA-N
Formula: C26H45NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 387.64

Physical Properties

Property code	Value	Unit	Source
gf	252.68	kJ/mol	Joback Method
hf	-399.96	kJ/mol	Joback Method
hfus	61.37	kJ/mol	Joback Method
hvap	85.20	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.802		Crippen Method
mcvol	364.990	ml/mol	McGowan Method
pc	898.02	kPa	Joback Method
rinpol	2854.00		NIST Webbook
tb	892.25	K	Joback Method
tc	1092.98	K	Joback Method
tf	504.12	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1204.80	J/mol×K	892.25	Joback Method
cpg	1225.16	J/mol×K	925.71	Joback Method
cpg	1244.32	J/mol×K	959.16	Joback Method
cpg	1262.34	J/mol×K	992.62	Joback Method
cpg	1279.30	J/mol×K	1026.07	Joback Method
cpg	1295.28	J/mol×K	1059.53	Joback Method
cpg	1310.33	J/mol×K	1092.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308572&Units=SI
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

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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