Benzamide, 4-butyl-N-(hept-2-yl)-

Inchi: InChI=1S/C18H29NO/c1-4-6-8-9-15(3)19-18(20)17-13-11-16(12-14-17)10-7-5-2/h11-15H
InchiKey: HOYVROFMCOGLJY-UHFFFAOYSA-N
Formula: C18H29NO
SMILES: CCCCCC(C)NC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 275.43

Physical Properties

Property code	Value	Unit	Source
gf	161.49	kJ/mol	Joback Method
hf	-254.18	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	71.39	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.728		Crippen Method
mcvol	252.270	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	746.50	K	Joback Method
tc	944.50	K	Joback Method
tf	419.15	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.07	J/mol×K	746.50	Joback Method
cpg	759.66	J/mol×K	779.50	Joback Method
cpg	776.22	J/mol×K	812.50	Joback Method
cpg	791.79	J/mol×K	845.50	Joback Method
cpg	806.42	J/mol×K	878.50	Joback Method
cpg	820.14	J/mol×K	911.50	Joback Method
cpg	833.01	J/mol×K	944.50	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=U407451&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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