Benzamide, 4-butyl-N-heptyl-

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

Physical Properties

Property code	Value	Unit	Source
gf	163.93	kJ/mol	Joback Method
hf	-248.90	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	71.78	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	4.729		Crippen Method
mcvol	252.270	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	746.94	K	Joback Method
tc	942.29	K	Joback Method
tf	434.15	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.56	J/mol×K	746.94	Joback Method
cpg	758.91	J/mol×K	779.50	Joback Method
cpg	775.26	J/mol×K	812.06	Joback Method
cpg	790.65	J/mol×K	844.61	Joback Method
cpg	805.14	J/mol×K	877.17	Joback Method
cpg	818.75	J/mol×K	909.73	Joback Method
cpg	831.54	J/mol×K	942.29	Joback Method

Sources

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=U407454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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