Benzamide, N-tetrahydrofurfuryl-4-butyl-

Inchi: InChI=1S/C16H23NO2/c1-2-3-5-13-7-9-14(10-8-13)16(18)17-12-15-6-4-11-19-15/h7-10,1
InchiKey: UDZMQMJZWXABFF-UHFFFAOYSA-N
Formula: C16H23NO2
SMILES: CCCCc1ccc(C(=O)NCC2CCCO2)cc1
Mol. weight [g/mol]: 261.36

Physical Properties

Property code	Value	Unit	Source
gf	97.52	kJ/mol	Joback Method
hf	-279.14	kJ/mol	Joback Method
hfus	39.46	kJ/mol	Joback Method
hvap	72.10	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	2.938		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	743.41	K	Joback Method
tc	963.09	K	Joback Method
tf	449.08	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.97	J/mol×K	743.41	Joback Method
cpg	670.47	J/mol×K	780.02	Joback Method
cpg	686.74	J/mol×K	816.64	Joback Method
cpg	701.84	J/mol×K	853.25	Joback Method
cpg	715.84	J/mol×K	889.86	Joback Method
cpg	728.80	J/mol×K	926.47	Joback Method
cpg	740.79	J/mol×K	963.09	Joback Method

Sources

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=U306989&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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