Benzamide, pentafluoro-N-(pentafluorobenzoyl)-N-butyl-

Inchi: InChI=1S/C18H9F10NO2/c1-2-3-4-29(17(30)5-7(19)11(23)15(27)12(24)8(5)20)18(31)6-9

InchiKey: ZHIDUFZTAONMNX-UHFFFAOYSA-N

Formula: C18H9F10NO2

SMILES: CCCCN(C(=O)c1c(F)c(F)c(F)c(F)c1F)C(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 461.25

Physical Properties

Property code	Value	Unit	Source
gf	-1865.96	kJ/mol	Joback Method
hf	-2175.22	kJ/mol	Joback Method
hfus	63.59	kJ/mol	Joback Method
hvap	74.20	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	5.160		Crippen Method
mcvol	247.780	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	1694.00		NIST Webbook
rinpol	1694.00		NIST Webbook
tb	827.28	K	Joback Method
tc	1014.45	K	Joback Method
tf	608.89	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.48	J/mol×K	827.28	Joback Method
cpg	729.75	J/mol×K	858.48	Joback Method
cpg	739.28	J/mol×K	889.67	Joback Method
cpg	748.09	J/mol×K	920.87	Joback Method
cpg	756.19	J/mol×K	952.06	Joback Method
cpg	763.59	J/mol×K	983.26	Joback Method
cpg	770.31	J/mol×K	1014.45	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=U407955&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