

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

Inchi: InChI=1S/C19H11F10NO2/c1-2-3-4-5-30(18(31)6-8(20)12(24)16(28)13(25)9(6)21)19(32)

InchiKey: PKDADNUMWBTFRJ-UHFFFAOYSA-N

Formula: C19H11F10NO2

SMILES: CCCCCN(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]: 475.28

Physical Properties

Property code	Value	Unit	Source
gf	-1857.54	kJ/mol	Joback Method
hf	-2195.86	kJ/mol	Joback Method
hfus	66.18	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	5.550		Crippen Method
mcvol	261.870	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinpol	1775.00		NIST Webbook
rinpol	1775.00		NIST Webbook
tb	850.16	K	Joback Method
tc	1041.22	K	Joback Method
tf	620.16	K	Joback Method
vc	1.093	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.93	J/mol×K	850.16	Joback Method
cpg	785.73	J/mol×K	882.00	Joback Method
cpg	795.73	J/mol×K	913.85	Joback Method
cpg	804.94	J/mol×K	945.69	Joback Method
cpg	813.37	J/mol×K	977.53	Joback Method
cpg	821.06	J/mol×K	1009.37	Joback Method
cpg	828.01	J/mol×K	1041.22	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=U407957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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