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

Inchi: InChI=1S/C20H13F10NO2/c1-2-3-4-5-6-31(19(32)7-9(21)13(25)17(29)14(26)10(7)22)20(

InchiKey: XNWDAVYFOCAMLC-UHFFFAOYSA-N

Formula: C20H13F10NO2

SMILES: CCCCCCN(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]: 489.31

Physical Properties

Property code	Value	Unit	Source
gf	-1849.12	kJ/mol	Joback Method
hf	-2216.50	kJ/mol	Joback Method
hfus	68.77	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-8.99		Crippen Method
logp	5.941		Crippen Method
mcvol	275.960	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	873.04	K	Joback Method
tc	1068.85	K	Joback Method
tf	631.43	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.26	J/mol×K	873.04	Joback Method
cpg	842.59	J/mol×K	905.67	Joback Method
cpg	853.04	J/mol×K	938.31	Joback Method
cpg	862.63	J/mol×K	970.94	Joback Method
cpg	871.39	J/mol×K	1003.58	Joback Method
cpg	879.33	J/mol×K	1036.21	Joback Method
cpg	886.48	J/mol×K	1068.85	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=U407959&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