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

Inchi: InChI=1S/C22H17F10NO2/c1-2-3-4-5-6-7-8-33(21(34)9-11(23)15(27)19(31)16(28)12(9)2

InchiKey: JRZDSJLLLOBONP-UHFFFAOYSA-N

Formula: C22H17F10NO2

SMILES: CCCCCCCCN(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]: 517.36

Physical Properties

Property code	Value	Unit	Source
gf	-1832.28	kJ/mol	Joback Method
hf	-2257.78	kJ/mol	Joback Method
hfus	73.95	kJ/mol	Joback Method
hvap	83.10	kJ/mol	Joback Method
log10ws	-9.83		Crippen Method
logp	6.721		Crippen Method
mcvol	304.140	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2056.00		NIST Webbook
tb	918.80	K	Joback Method
tc	1127.01	K	Joback Method
tf	653.97	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.26	J/mol×K	918.80	Joback Method
cpg	958.67	J/mol×K	953.50	Joback Method
cpg	970.02	J/mol×K	988.20	Joback Method
cpg	980.35	J/mol×K	1022.91	Joback Method
cpg	989.69	J/mol×K	1057.61	Joback Method
cpg	998.07	J/mol×K	1092.31	Joback Method
cpg	1005.52	J/mol×K	1127.01	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=U407960&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