

Benzamide, pentafluoro-N-(pentafluorobenzoyl)-N-3-methylbu

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

InchiKey: YPAMBHXPKREJHR-UHFFFAOYSA-N

Formula: C19H11F10NO2

SMILES: CC(C)CCN(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	-1859.98	kJ/mol	Joback Method
hf	-2201.14	kJ/mol	Joback Method
hfus	62.65	kJ/mol	Joback Method
hvap	76.04	kJ/mol	Joback Method
log10ws	-8.33		Crippen Method
logp	5.406		Crippen Method
mcvol	261.870	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
tb	849.72	K	Joback Method
tc	1041.07	K	Joback Method
tf	605.16	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.51	J/molxK	849.72	Joback Method
cpg	786.31	J/molxK	881.61	Joback Method
cpg	796.30	J/molxK	913.50	Joback Method
cpg	805.49	J/molxK	945.39	Joback Method
cpg	813.89	J/molxK	977.28	Joback Method
cpg	821.53	J/molxK	1009.18	Joback Method
cpg	828.43	J/molxK	1041.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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