

Benzoic acid, 2-(pentafluoropropionylamino)-

Inchi:	InChI=1S/C10H6F5NO3/c11-9(12,10(13,14)15)8(19)16-6-4-2-1-3-5(6)7(17)18/h1-4H,(H,
InchiKey:	ZRZUVSMZTNXVFZ-UHFFFAOYSA-N
Formula:	C10H6F5NO3
SMILES:	O=C(O)c1ccccc1NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	283.15
CAS:	64995-47-7

Physical Properties

Property code	Value	Unit	Source
gf	-1137.54	kJ/mol	Joback Method
hf	-1346.64	kJ/mol	Joback Method
hfus	28.27	kJ/mol	Joback Method
hvap	70.72	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.521		Crippen Method
mvol	155.840	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1544.00		NIST Webbook
rinpol	1544.00		NIST Webbook
tb	699.84	K	Joback Method
tc	889.23	K	Joback Method
tf	462.53	K	Joback Method
vc	0.622	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.20	J/molxK	699.84	Joback Method
cpg	439.17	J/molxK	731.41	Joback Method
cpg	446.47	J/molxK	762.97	Joback Method
cpg	453.16	J/molxK	794.54	Joback Method
cpg	459.30	J/molxK	826.10	Joback Method
cpg	464.94	J/molxK	857.67	Joback Method
cpg	470.12	J/molxK	889.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64995477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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