Benzoic acid, 4-(pentafluoropropionylamino)-

Inchi: InChI=1S/C10H6F5NO3/c11-9(12,10(13,14)15)8(19)16-6-3-1-5(2-4-6)7(17)18/h1-4H,(H,1
InchiKey: ZQDHKYUQWHFJRN-UHFFFAOYSA-N
Formula: C10H6F5NO3
SMILES: O=C(O)c1ccc(NC(=O)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 283.15
CAS: 882828-33-3

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
mcvol	155.840	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
tb	699.84	K	Joback Method
tc	889.23	K	Joback Method
tf	462.53	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.20	J/mol×K	699.84	Joback Method
cpg	439.17	J/mol×K	731.41	Joback Method
cpg	446.47	J/mol×K	762.97	Joback Method
cpg	453.16	J/mol×K	794.54	Joback Method
cpg	459.30	J/mol×K	826.10	Joback Method
cpg	464.94	J/mol×K	857.67	Joback Method
cpg	470.12	J/mol×K	889.23	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=C882828333&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