Methyl 2-(N-pentafluoropropionylamino)benzoate

Inchi: InChI=1S/C11H8F5NO3/c1-20-8(18)6-4-2-3-5-7(6)17-9(19)10(12,13)11(14,15)16/h2-5H,
InchiKey: WQHFQGJRFWCNTG-UHFFFAOYSA-N
Formula: C11H8F5NO3
SMILES: COC(=O)c1ccccc1NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 297.18

Physical Properties

Property code	Value	Unit	Source
gf	-1097.30	kJ/mol	Joback Method
hf	-1347.27	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	58.68	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.609		Crippen Method
mcvol	169.930	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1411.00		NIST Webbook
rinpol	1411.00		NIST Webbook
tb	652.96	K	Joback Method
tc	847.74	K	Joback Method
tf	435.21	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.34	J/mol×K	652.96	Joback Method
cpg	469.04	J/mol×K	685.42	Joback Method
cpg	478.91	J/mol×K	717.89	Joback Method
cpg	488.01	J/mol×K	750.35	Joback Method
cpg	496.37	J/mol×K	782.81	Joback Method
cpg	504.04	J/mol×K	815.28	Joback Method
cpg	511.08	J/mol×K	847.74	Joback Method

Sources

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=U374367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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