

Methyl 3-(N-pentafluoropropionylamino)benzoate

Inchi:	InChI=1S/C11H8F5NO3/c1-20-8(18)6-3-2-4-7(5-6)17-9(19)10(12,13)11(14,15)16/h2-5H,
InchiKey:	XDEMMFMXYWTUFR-UHFFFAOYSA-N
Formula:	C11H8F5NO3
SMILES:	<chem>COC(=O)c1cccc(NC(=O)C(F)(F)C(F)(F)F)c1</chem>
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
rinqol	1506.00		NIST Webbook
tb	652.96	K	Joback Method
tc	847.74	K	Joback Method
tf	435.21	K	Joback Method
vc	0.676	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374363&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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

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