Nitrobenzene, 3-pentafluoropropionylamino-4-pentafluoropropio

Inchi: InChI=1S/C12H4F10N2O5/c13-9(14,11(17,18)19)7(25)23-5-3-4(24(27)28)1-2-6(5)29-8(2

InchiKey: GXNJMXJHKSHDGC-UHFFFAOYSA-N

Formula: C12H4F10N2O5

SMILES: O=C(Nc1cc([N+](=O)[O-])ccc1OC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 446.15

Physical Properties

Property code	Value	Unit	Source
gf	-2031.33	kJ/mol	Joback Method
hf	-2388.19	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	71.48	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	3.834		Crippen Method
mcvol	210.290	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	1475.00		NIST Webbook
tb	822.55	K	Joback Method
tc	1022.51	K	Joback Method
tf	610.40	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.41	J/mol×K	822.55	Joback Method
cpg	646.42	J/mol×K	855.88	Joback Method
cpg	652.75	J/mol×K	889.20	Joback Method
cpg	658.49	J/mol×K	922.53	Joback Method
cpg	663.73	J/mol×K	955.86	Joback Method
cpg	668.56	J/mol×K	989.18	Joback Method
cpg	673.06	J/mol×K	1022.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374264&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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