2-((2,2,3,3,3-Pentafluoropropanoyl)amino)phenyl 2,2,3,3,3-pentafluoropropanoate

Inchi: InChI=1S/C12H5F10NO3/c13-9(14,11(17,18)19)7(24)23-5-3-1-2-4-6(5)26-8(25)10(15,16
InchiKey: METVPIHLLFECEQ-UHFFFAOYSA-N
Formula: C12H5F10NO3
SMILES: O=C(Nc1ccccc1OC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 401.16

Physical Properties

Property code	Value	Unit	Source
gf	-2057.25	kJ/mol	Joback Method
hf	-2365.96	kJ/mol	Joback Method
hfus	31.12	kJ/mol	Joback Method
hvap	54.23	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.926		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1166.00		NIST Webbook
tb	665.73	K	Joback Method
tc	841.75	K	Joback Method
tf	454.27	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.73	J/mol×K	665.73	Joback Method
cpg	564.35	J/mol×K	695.07	Joback Method
cpg	573.15	J/mol×K	724.40	Joback Method
cpg	581.18	J/mol×K	753.74	Joback Method
cpg	588.50	J/mol×K	783.08	Joback Method
cpg	595.19	J/mol×K	812.42	Joback Method
cpg	601.29	J/mol×K	841.75	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=U373482&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

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