N-(2,6-Diethylphenyl)-2,2,3,3,3-pentafluoropropan

Other names: 2-Pentafluoro-n-propionylamino-1,3-diethylbenzene
2,6-Diethylaniline, N-pentafluoropropionyl-
Inchi: InChI=1S/C13H14F5NO/c1-3-8-6-5-7-9(4-2)10(8)19-11(20)12(14,15)13(16,17)18/h5-7H,
InchiKey: GLEAQAVYZLTCJB-UHFFFAOYSA-N
Formula: C13H14F5NO
SMILES: CCc1cccc(CC)c1NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 295.25

Physical Properties

Property code	Value	Unit	Source
gf	-856.17	kJ/mol	Joback Method
hf	-1155.22	kJ/mol	Joback Method
hfus	29.96	kJ/mol	Joback Method
hvap	54.64	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.948		Crippen Method
mcvol	190.670	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	627.41	K	Joback Method
tc	813.12	K	Joback Method
tf	398.11	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.04	J/mol×K	627.41	Joback Method
cpg	529.36	J/mol×K	658.36	Joback Method
cpg	541.80	J/mol×K	689.31	Joback Method
cpg	553.42	J/mol×K	720.27	Joback Method
cpg	564.26	J/mol×K	751.22	Joback Method
cpg	574.38	J/mol×K	782.17	Joback Method

cpg	583.83	J/mol×K	813.12	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373375&Units=SI

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