N-Phenylperfluorobenzamide

Other names: 2,3,4,5,6-Pentafluoro-N-phenylbenzamide
Inchi: InChI=1S/C13H6F5NO/c14-8-7(9(15)11(17)12(18)10(8)16)13(20)19-6-4-2-1-3-5-6/h1-5H
InchiKey: WRYTWJSCSKBXDY-UHFFFAOYSA-N
Formula: C13H6F5NO
SMILES: O=C(Nc1ccccc1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 287.18
CAS: 58627-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-778.33	kJ/mol	Joback Method
hf	-935.60	kJ/mol	Joback Method
hfus	37.66	kJ/mol	Joback Method
hvap	61.49	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.634		Crippen Method
mcvol	166.910	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
tb	675.49	K	Joback Method
tc	878.28	K	Joback Method
tf	457.25	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.26	J/mol×K	675.49	Joback Method
cpg	435.75	J/mol×K	709.29	Joback Method
cpg	445.52	J/mol×K	743.09	Joback Method
cpg	454.61	J/mol×K	776.88	Joback Method
cpg	463.04	J/mol×K	810.68	Joback Method
cpg	470.82	J/mol×K	844.48	Joback Method
cpg	477.98	J/mol×K	878.28	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=C58627193&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume