Heptafluorobutanamide, N-(2-fluorophenyl)-

Inchi: InChI=1S/C10H5F8NO/c11-5-3-1-2-4-6(5)19-7(20)8(12,13)9(14,15)10(16,17)18/h1-4H,(H
InchiKey: MHBXYDUAIKHVSN-UHFFFAOYSA-N
Formula: C10H5F8NO
SMILES: O=C(Nc1ccccc1F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 307.14

Physical Properties

Property code	Value	Unit	Source
gf	-1453.39	kJ/mol	Joback Method
hf	-1678.91	kJ/mol	Joback Method
hfus	24.40	kJ/mol	Joback Method
hvap	43.55	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.597		Crippen Method
mcvol	153.710	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	642.00		NIST Webbook
rinpol	642.00		NIST Webbook
tb	548.37	K	Joback Method
tc	724.47	K	Joback Method
tf	355.97	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.93	J/mol×K	548.37	Joback Method
cpg	411.10	J/mol×K	577.72	Joback Method
cpg	421.37	J/mol×K	607.07	Joback Method
cpg	430.81	J/mol×K	636.42	Joback Method
cpg	439.46	J/mol×K	665.77	Joback Method
cpg	447.39	J/mol×K	695.12	Joback Method
cpg	454.65	J/mol×K	724.47	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=U308268&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