Propanamide, N-(4-fluorophenyl)-2,2,3,3,3-pentafluoro-

Inchi: InChI=1S/C9H5F6NO/c10-5-1-3-6(4-2-5)16-7(17)8(11,12)9(13,14)15/h1-4H,(H,16,17)
InchiKey: PBUZXWZWAZFUOL-UHFFFAOYSA-N
Formula: C9H5F6NO
SMILES: O=C(Nc1ccc(F)cc1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 257.13
CAS: 959055-29-9

Physical Properties

Property code	Value	Unit	Source
gf	-1075.03	kJ/mol	Joback Method
hf	-1257.30	kJ/mol	Joback Method
hfus	23.07	kJ/mol	Joback Method
hvap	44.25	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.962		Crippen Method
mcvol	136.080	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	885.00		NIST Webbook
rinpol	885.00		NIST Webbook
tb	530.18	K	Joback Method
tc	714.58	K	Joback Method
tf	341.10	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.81	J/mol×K	530.18	Joback Method
cpg	345.65	J/mol×K	560.91	Joback Method
cpg	355.67	J/mol×K	591.65	Joback Method
cpg	364.91	J/mol×K	622.38	Joback Method
cpg	373.41	J/mol×K	653.11	Joback Method
cpg	381.23	J/mol×K	683.84	Joback Method
cpg	388.42	J/mol×K	714.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959055299&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