Propanamide, N-(3-nitrophenyl)-2,2,3,3,3-pentafluoro-

Inchi: InChI=1S/C9H5F5N2O3/c10-8(11,9(12,13)14)7(17)15-5-2-1-3-6(4-5)16(18)19/h1-4H,(H,1

InchiKey: TUGCGBHNKPWBKD-UHFFFAOYSA-N

Formula: C9H5F5N2O3

SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 284.14

Physical Properties

Property code	Value	Unit	Source
gf	-844.67	kJ/mol	Joback Method
hf	-1071.95	kJ/mol	Joback Method
hfus	31.35	kJ/mol	Joback Method
hvap	61.66	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.731		Crippen Method
mcvol	151.730	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1504.00		NIST Webbook
tb	682.75	K	Joback Method
tc	899.86	K	Joback Method
tf	484.12	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.77	J/mol×K	682.75	Joback Method
cpg	424.97	J/mol×K	718.94	Joback Method
cpg	433.28	J/mol×K	755.12	Joback Method
cpg	440.79	J/mol×K	791.31	Joback Method
cpg	447.57	J/mol×K	827.49	Joback Method
cpg	453.71	J/mol×K	863.68	Joback Method
cpg	459.30	J/mol×K	899.86	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=U307335&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