Butanamide, N-(3-nitrophenyl)-2,2,3,3,4,4,4-heptafluoro-

Inchi: InChI=1S/C10H5F7N2O3/c11-8(12,9(13,14)10(15,16)17)7(20)18-5-2-1-3-6(4-5)19(21)22

InchiKey: XLJRHHILGOGNKM-UHFFFAOYSA-N

Formula: C10H5F7N2O3

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

Mol. weight [g/mol]: 334.15

Physical Properties

Property code	Value	Unit	Source
gf	-1223.03	kJ/mol	Joback Method
hf	-1493.56	kJ/mol	Joback Method
hfus	32.68	kJ/mol	Joback Method
hvap	60.96	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.366		Crippen Method
mcvol	169.360	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1531.00		NIST Webbook
tb	700.94	K	Joback Method
tc	908.17	K	Joback Method
tf	498.99	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.08	J/mol×K	700.94	Joback Method
cpg	493.12	J/mol×K	735.48	Joback Method
cpg	501.26	J/mol×K	770.02	Joback Method
cpg	508.61	J/mol×K	804.55	Joback Method
cpg	515.25	J/mol×K	839.09	Joback Method
cpg	521.28	J/mol×K	873.63	Joback Method
cpg	526.81	J/mol×K	908.17	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=U307281&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