N-(3-Chlorophenyl)-2,2,3,3,4,4,4-heptafluorobutan

Other names: Butanamide, N-(3-chlorophenyl)-2,2,3,3,4,4,4-heptafluoro-
Inchi: InChI=1S/C10H5ClF7NO/c11-5-2-1-3-6(4-5)19-7(20)8(12,13)9(14,15)10(16,17)18/h1-4H
InchiKey: UJBGCMKVPMWSOM-UHFFFAOYSA-N
Formula: C10H5ClF7NO
SMILES: O=C(Nc1cccc(Cl)c1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 323.60
CAS: 106376-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-1270.51	kJ/mol	Joback Method
hf	-1498.54	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	48.75	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.111		Crippen Method
mcvol	164.180	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1332.00		NIST Webbook
tb	586.53	K	Joback Method
tc	775.18	K	Joback Method
tf	385.30	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.45	J/mol×K	586.53	Joback Method
cpg	427.96	J/mol×K	617.97	Joback Method
cpg	437.53	J/mol×K	649.41	Joback Method
cpg	446.24	J/mol×K	680.86	Joback Method
cpg	454.15	J/mol×K	712.30	Joback Method

cpg	461.35	J/mol×K	743.74	Joback Method
cpg	467.88	J/mol×K	775.18	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106376367&Units=SI

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

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