Benzamide, N-(3-chlorophenyl)-2,6-difluoro-

Inchi: InChI=1S/C13H8ClF2NO/c14-8-3-1-4-9(7-8)17-13(18)12-10(15)5-2-6-11(12)16/h1-7H,(H
InchiKey: LZWCYTYURGFFOM-UHFFFAOYSA-N
Formula: C13H8ClF2NO
SMILES: O=C(Nc1cccc(Cl)c1)c1c(F)cccc1F
Mol. weight [g/mol]: 267.66

Physical Properties

Property code	Value	Unit	Source
gf	-186.57	kJ/mol	Joback Method
hf	-340.07	kJ/mol	Joback Method
hfus	33.40	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.870		Crippen Method
mcvol	173.840	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
tb	705.15	K	Joback Method
tc	936.96	K	Joback Method
tf	460.36	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.65	J/mol×K	705.15	Joback Method
cpg	438.02	J/mol×K	743.78	Joback Method
cpg	448.45	J/mol×K	782.42	Joback Method
cpg	458.01	J/mol×K	821.05	Joback Method
cpg	466.73	J/mol×K	859.69	Joback Method
cpg	474.67	J/mol×K	898.32	Joback Method
cpg	481.87	J/mol×K	936.96	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=U307429&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