Benzamide, N-(3-chlorophenyl)-4-fluoro-

Inchi: InChI=1S/C13H9ClFNO/c14-10-2-1-3-12(8-10)16-13(17)9-4-6-11(15)7-5-9/h1-8H,(H,16,1
InchiKey: XUEQQRMECUEOSZ-UHFFFAOYSA-N
Formula: C13H9ClFNO
SMILES: O=C(Nc1cccc(Cl)c1)c1ccc(F)cc1
Mol. weight [g/mol]: 249.67

Physical Properties

Property code	Value	Unit	Source
gf	17.87	kJ/mol	Joback Method
hf	-132.49	kJ/mol	Joback Method
hfus	30.71	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.731		Crippen Method
mcvol	172.070	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
tb	700.90	K	Joback Method
tc	942.60	K	Joback Method
tf	447.25	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.15	J/mol×K	700.90	Joback Method
cpg	432.28	J/mol×K	741.18	Joback Method
cpg	443.38	J/mol×K	781.47	Joback Method
cpg	453.49	J/mol×K	821.75	Joback Method
cpg	462.69	J/mol×K	862.03	Joback Method
cpg	471.04	J/mol×K	902.32	Joback Method
cpg	478.60	J/mol×K	942.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307103&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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