Benzamide, 3-chloro-2-fluoro-N-methyl-

Inchi: InChI=1S/C8H7ClFNO/c1-11-8(12)5-3-2-4-6(9)7(5)10/h2-4H,1H3,(H,11,12)
InchiKey: XPWCHFCRQGESMV-UHFFFAOYSA-N
Formula: C8H7ClFNO
SMILES: CNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 187.60

Physical Properties

Property code	Value	Unit	Source
gf	-136.64	kJ/mol	Joback Method
hf	-265.82	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.839		Crippen Method
mcvol	125.380	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
tb	559.82	K	Joback Method
tc	777.97	K	Joback Method
tf	364.48	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.35	J/mol×K	559.82	Joback Method
cpg	275.34	J/mol×K	596.18	Joback Method
cpg	284.71	J/mol×K	632.54	Joback Method
cpg	293.46	J/mol×K	668.90	Joback Method
cpg	301.62	J/mol×K	705.26	Joback Method
cpg	309.21	J/mol×K	741.62	Joback Method
cpg	316.25	J/mol×K	777.97	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=U407817&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