3,4-Dichlorobenzamide

Inchi: InChI=1S/C7H5Cl2NO/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3H,(H2,10,11)
InchiKey: XURBWYCGQQXTHJ-UHFFFAOYSA-N
Formula: C7H5Cl2NO
SMILES: NC(=O)c1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 190.03
CAS: 2670-38-4

Physical Properties

Property code	Value	Unit	Source
gf	14.88	kJ/mol	Joback Method
hf	-84.49	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	60.93	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.092		Crippen Method
mcvol	121.760	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
tb	597.46	K	Joback Method
tc	845.33	K	Joback Method
tf	413.14	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.93	J/mol×K	597.46	Joback Method
cpg	249.24	J/mol×K	638.77	Joback Method
cpg	256.89	J/mol×K	680.08	Joback Method
cpg	263.93	J/mol×K	721.39	Joback Method
cpg	270.37	J/mol×K	762.70	Joback Method
cpg	276.25	J/mol×K	804.01	Joback Method
cpg	281.60	J/mol×K	845.33	Joback Method

Sources

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=C2670384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume