Benzenesulfonamide, 4-amino-N-(3,4-dichlorophenyl)-

Other names: 4-Amino-N-(3,4-chlorophenyl)benzene sulfonamide
Inchi: InChI=1S/C12H10Cl2N2O2S/c13-11-6-3-9(7-12(11)14)16-19(17,18)10-4-1-8(15)2-5-10/h
InchiKey: CDCMAMVXGZBIAX-UHFFFAOYSA-N
Formula: C12H10Cl2N2O2S
SMILES: Nc1ccc(S(=O)(=O)Nc2ccc(Cl)c(Cl)c2)cc1
Mol. weight [g/mol]: 317.19
CAS: 34392-63-7

Physical Properties

Property code	Value	Unit	Source
gf	-90.47	kJ/mol	Joback Method
hf	-249.93	kJ/mol	Joback Method
hfus	43.82	kJ/mol	Joback Method
hsub	167.50 ± 3.60	kJ/mol	NIST Webbook
hvap	136.70	kJ/mol	NIST Webbook
log10ws	-3.98		Crippen Method
logp	3.376		Crippen Method
mcvol	204.950	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
tb	787.60	K	Joback Method
tc	1036.29	K	Joback Method
tf	549.72	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.20	J/mol×K	994.84	Joback Method
cpg	508.62	J/mol×K	787.60	Joback Method
cpg	519.25	J/mol×K	829.05	Joback Method
cpg	528.69	J/mol×K	870.50	Joback Method
cpg	536.97	J/mol×K	911.94	Joback Method
cpg	544.13	J/mol×K	953.39	Joback Method
cpg	555.22	J/mol×K	1036.29	Joback Method

hfust	51.50	kJ/mol	497.90	NIST Webbook
hsubt	161.40 ± 3.60	kJ/mol	433.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34392637&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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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