

3',4',4-Trichlorobenzene sulfonanilide

Inchi:	InChI=1S/C12H8Cl3NO2S/c13-8-1-4-10(5-2-8)19(17,18)16-9-3-6-11(14)12(15)7-9/h1-7,1
InchiKey:	TUHPMTANLYSLFD-UHFFFAOYSA-N
Formula:	C12H8Cl3NO2S
SMILES:	O=S(=O)(Nc1ccc(Cl)c(Cl)c1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	336.62
CAS:	7454-52-6

Physical Properties

Property code	Value	Unit	Source
gf	-168.85	kJ/mol	Joback Method
hf	-299.46	kJ/mol	Joback Method
hfus	42.82	kJ/mol	Joback Method
hvap	87.07	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.448		Crippen Method
mcvol	207.210	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	752.50	K	Joback Method
tc	999.00	K	Joback Method
tf	496.38	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.76	J/molxK	752.50	Joback Method
cpg	486.39	J/molxK	793.58	Joback Method
cpg	495.87	J/molxK	834.67	Joback Method
cpg	504.25	J/molxK	875.75	Joback Method
cpg	511.55	J/molxK	916.83	Joback Method
cpg	517.81	J/molxK	957.92	Joback Method
cpg	523.06	J/molxK	999.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7454526&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

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

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