2,4-Dichloro-1-naphthyl 4-chlorobenzenesulfonate

Inchi: InChI=1S/C16H9Cl3O3S/c17-10-5-7-11(8-6-10)23(20,21)22-16-13-4-2-1-3-12(13)14(18)9

InchiKey: DNNCQNJRNQSPCT-UHFFFAOYSA-N

Formula: C16H9Cl3O3S

SMILES: O=S(=O)(Oc1c(Cl)cc(Cl)c2ccccc12)c1ccc(Cl)cc1

Mol. weight [g/mol]: 387.67

CAS: 19361-91-2

Physical Properties

Property code	Value	Unit	Source
gf	-232.54	kJ/mol	Joback Method
hf	-388.11	kJ/mol	Joback Method
hfus	45.90	kJ/mol	Joback Method
hvap	94.25	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.568		Crippen Method
mcvol	240.000	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	840.23	K	Joback Method
tc	1093.35	K	Joback Method
tf	556.25	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.75	J/mol×K	840.23	Joback Method
cpg	595.01	J/mol×K	882.42	Joback Method
cpg	604.05	J/mol×K	924.60	Joback Method
cpg	611.92	J/mol×K	966.79	Joback Method
cpg	618.68	J/mol×K	1008.97	Joback Method
cpg	624.38	J/mol×K	1051.16	Joback Method
cpg	629.08	J/mol×K	1093.35	Joback Method

Sources

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=C19361912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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