

Aniline, 4-(n,n-dimethylamino)-2-(3,4-dimethylphenylsulfo

Inchi: InChI=1S/C16H20N2O2S/c1-11-5-7-14(9-12(11)2)21(19,20)16-10-13(18(3)4)6-8-15(16)1

InchiKey: MHSIKLXGOJINBL-UHFFFAOYSA-N

Formula: C16H20N2O2S

SMILES: Cc1ccc(S(=O)(=O)c2cc(N(C)C)ccc2N)cc1C

Mol. weight [g/mol]: 304.41

CAS: 19770-82-2

Physical Properties

Property code	Value	Unit	Source
gf	-21.17	kJ/mol	Joback Method
hf	-298.42	kJ/mol	Joback Method
hfus	43.32	kJ/mol	Joback Method
hvap	89.73	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.784		Crippen Method
mcvol	236.830	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
tb	771.51	K	Joback Method
tc	998.13	K	Joback Method
tf	527.29	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.28	J/mol×K	771.51	Joback Method
cpg	679.71	J/mol×K	809.28	Joback Method
cpg	693.86	J/mol×K	847.05	Joback Method
cpg	706.76	J/mol×K	884.82	Joback Method
cpg	718.46	J/mol×K	922.59	Joback Method
cpg	728.98	J/mol×K	960.36	Joback Method
cpg	738.36	J/mol×K	998.13	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=C19770822&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

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