

Acetamide, N-[4-[(4-aminophenyl)sulfonyl]phenyl]-

Other names:

N-Acetyl-4,4'-diaminodiphenylsulfone
Acetanilide, 4'-sulfanilyl-
Acetyldapsone
N-Acetyldapsone
MADDS
Monoacetyldapsone
4'-Sulfanilylacetanilide
N-(4-[(4-Aminophenyl)sulfonyl]phenyl)acetamide
NSC 27184
4-Acetylamino-4'-aminodiphenyl sulfone

Inchi: InChI=1S/C14H14N2O3S/c1-10(17)16-12-4-8-14(9-5-12)20(18,19)13-6-2-11(15)3-7-13/h

InchiKey: WDOCBIHNYQINH-UHFFFAOYSA-N

Formula: C14H14N2O3S

SMILES: CC(=O)Nc1ccc(S(=O)(=O)c2ccc(N)cc2)cc1

Mol. weight [g/mol]: 290.34

CAS: 565-20-8

Physical Properties

Property code	Value	Unit	Source
gf	-169.06	kJ/mol	Joback Method
hf	-360.84	kJ/mol	Joback Method
hfus	42.59	kJ/mol	Joback Method
hvap	95.09	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.060		Crippen Method
mcvol	210.220	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
tb	807.39	K	Joback Method
tc	1046.78	K	Joback Method
tf	549.83	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.74	J/mol×K	807.39	Joback Method
cpg	594.83	J/mol×K	847.29	Joback Method
cpg	605.64	J/mol×K	887.19	Joback Method
cpg	615.20	J/mol×K	927.08	Joback Method
cpg	623.55	J/mol×K	966.98	Joback Method
cpg	630.74	J/mol×K	1006.88	Joback Method
cpg	636.79	J/mol×K	1046.78	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=C565208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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