MAFENIDE

Other names: 4-(Aminomethyl)benzenesulfonamide
4-Homosulfanilamide
Ambamide
Benzamsulfonamide
Benzenesulfonamide, 4-(aminomethyl)-
Emilene
Homonal
Homosul
Homosulfanilamide
Malfamin
Maphenid
Maphenide
Marprontil
Mesudin
Mesudrin
NSC-34632
Neofamid
Paramenyl
Septicid
Sulfamylon
p-(Aminomethyl)benzenesulfonamide
p-Toluenesulfonamide, «alpha»-amino-
«alpha»-Amino-p-toluenesulfonamide

Inchi: InChI=1S/C7H10N2O2S/c8-5-6-1-3-7(4-2-6)12(9,10)11/h1-4H,5,8H2,(H2,9,10,11)

InchiKey: TYMRLRRVMHJFTF-UHFFFAOYSA-N

Formula: C7H10N2O2S

SMILES: NCc1ccc(S(N)(=O)=O)cc1

Mol. weight [g/mol]: 186.24

Physical Properties

Property code	Value	Unit	Source
hf	-251.58	kJ/mol	Cheméo Relay (1.0)
hfus	29.31	kJ/mol	Joback Method
hvap	94.96	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	-1.77		Cheméo Relay (1.0)

logp	-0.207		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
tb	600.84	K	Cheméo Relay (1.0)
tf	406.18	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.34	J/mol×K	584.06	Joback Method
cpg	326.12	J/mol×K	622.15	Joback Method
cpg	337.07	J/mol×K	660.23	Joback Method
cpg	347.21	J/mol×K	698.32	Joback Method
cpg	356.55	J/mol×K	736.40	Joback Method
cpg	365.10	J/mol×K	774.49	Joback Method
cpg	372.87	J/mol×K	812.58	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C138396&Units=SI
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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point