Sulfabenzamide

Other names:	Benzamide, N-[(4-aminophenyl)sulfonyl]-
	Benzamide, N-sulfanilyl-
	N1-Benzoylsulfanilamide
	N-(p-Aminobenzenesulfonyl)benzamide
	N-Sulfanilylbenzamide
	Sulfabenzamid
	Sulfabenzid
	Sulfabenzide
	Sulfabenzoylamide
	Sulfanilamide, N1-benzoyl-
	N-((4-Aminophenyl)sulfonyl)benzamide
	NSC 74587
	N-Sulfamylbenzamide
	4-Amino-N-benzoylbenzenesulfonamide
	Trysul
	Sultrin
Inchi:	InChI=1S/C13H12N2O3S/c14-11-6-8-12(9-7-11)19(17,18)15-13(16)10-4-2-1-3-5-10/h1-9
InchiKey:	PBCZLFBEBARBBI-UHFFFAOYSA-N
Formula:	C13H12N2O3S
SMILES:	Nc1ccc(S(=O)(=O)NC(=O)c2ccccc2)cc1
Mol. weight [g/mol]:	276.31
CAS:	127-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-167.85	kJ/mol	Joback Method
hf	-328.73	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	92.20	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	1.387		Crippen Method
mcvol	196.130	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
rinpol	2863.00		NIST Webbook
rinpol	2863.00		NIST Webbook
tb	779.53	K	Joback Method
tc	1022.62	K	Joback Method

tf	526.04	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.90	J/mol×K	779.53	Joback Method
cpg	542.87	J/mol×K	820.05	Joback Method
cpg	553.54	J/mol×K	860.56	Joback Method
cpg	562.96	J/mol×K	901.08	Joback Method
cpg	571.19	J/mol×K	941.59	Joback Method
cpg	578.26	J/mol×K	982.11	Joback Method
cpg	584.23	J/mol×K	1022.62	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C127719&Units=SI

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume