S-(2-([3-(phenylsulfanyl)propyl]amino)ethyl) hydrogen thiosulfate

Inchi: InChI=1S/C11H17NO3S3/c13-18(14,15)17-10-8-12-7-4-9-16-11-5-2-1-3-6-11/h1-3,5-6,12

InchiKey: TUJWDXKDMJKBBV-UHFFFAOYSA-N

Formula: C11H17NO3S3

SMILES: O=S(=O)(O)SCCNCCCSc1ccccc1

Mol. weight [g/mol]: 307.45

CAS: 20748-26-9

Physical Properties

Property code	Value	Unit	Source
gf	-295.58	kJ/mol	Joback Method
hf	-502.21	kJ/mol	Joback Method
hfus	47.11	kJ/mol	Joback Method
hvap	97.74	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.294		Crippen Method
mcvol	218.730	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
tb	805.45	K	Joback Method
tc	1020.01	K	Joback Method
tf	460.99	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.55	J/mol×K	805.45	Joback Method
cpg	609.68	J/mol×K	841.21	Joback Method
cpg	619.73	J/mol×K	876.97	Joback Method
cpg	628.71	J/mol×K	912.73	Joback Method
cpg	636.65	J/mol×K	948.49	Joback Method
cpg	643.56	J/mol×K	984.25	Joback Method
cpg	649.44	J/mol×K	1020.01	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=C20748269&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