Bis(2-diethylaminoethyl) sulfide

Other names: 2,2'-Thiodi(ethanamine), N,N,N',N'-tetraethyl-
Inchi: InChI=1S/C12H28N2S/c1-5-13(6-2)9-11-15-12-10-14(7-3)8-4/h5-12H2,1-4H3
InchiKey: LYFNBXZVKYDWNX-UHFFFAOYSA-N
Formula: C12H28N2S
SMILES: CCN(CC)CCSCCN(CC)CC
Mol. weight [g/mol]: 232.43
CAS: 6006-58-2

Physical Properties

Property code	Value	Unit	Source
gf	304.84	kJ/mol	Joback Method
hf	-114.08	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	53.21	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	2.403		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1579.00		NIST Webbook
tb	567.62	K	Joback Method
tc	742.69	K	Joback Method
tf	324.34	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.39	J/mol×K	567.62	Joback Method
cpg	565.49	J/mol×K	596.80	Joback Method

cpg	582.74	J/mol×K	625.98	Joback Method
cpg	599.18	J/mol×K	655.16	Joback Method
cpg	614.83	J/mol×K	684.33	Joback Method
cpg	629.72	J/mol×K	713.51	Joback Method
cpg	643.87	J/mol×K	742.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6006582&Units=SI
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

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