Ethane, 1,2-bis-(2-diethylamonoethylthio)

Other names: Ethane, 1,2-bis-(2-diethylaminoethylthio)
Inchi: InChI=1S/C14H32N2S2/c1-5-15(6-2)9-11-17-13-14-18-12-10-16(7-3)8-4/h5-14H2,1-4H3
InchiKey: VUBCXWHBJHMDBK-UHFFFAOYSA-N
Formula: C14H32N2S2
SMILES: CCN(CC)CCSCCSCCN(CC)CC
Mol. weight [g/mol]: 292.55

Physical Properties

Property code	Value	Unit	Source
gf	354.80	kJ/mol	Joback Method
hf	-113.49	kJ/mol	Joback Method
hfus	46.32	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	3.136		Crippen Method
mcvol	260.780	ml/mol	McGowan Method
pc	1559.81	kPa	Joback Method
rinpol	2018.00		NIST Webbook
rinpol	2018.00		NIST Webbook
rinpol	2021.00		NIST Webbook
rinpol	2021.00		NIST Webbook
rinpol	2021.00		NIST Webbook
tb	682.16	K	Joback Method
tc	869.45	K	Joback Method
tf	381.28	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.13	J/mol×K	682.16	Joback Method
cpg	742.68	J/mol×K	713.38	Joback Method
cpg	760.25	J/mol×K	744.59	Joback Method
cpg	776.85	J/mol×K	775.81	Joback Method

cpg	792.53	J/mol×K	807.02	Joback Method
cpg	807.32	J/mol×K	838.24	Joback Method
cpg	821.24	J/mol×K	869.45	Joback Method

Sources

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=R334859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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