Bis(diisopropylaminoethyl)disulfide

Other names: Disulfane, bis(2-diisopropylaminoethyl)-
bis-[2-(Diisopropylamino)ethyl]disulfide
Inchi: InChI=1S/C16H36N2S2/c1-13(2)17(14(3)4)9-11-19-20-12-10-18(15(5)6)16(7)8/h13-16H,
InchiKey: ZZTNOKXWKFKVLW-UHFFFAOYSA-N
Formula: C16H36N2S2
SMILES: CC(C)N(CCSSCCN(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]: 320.60
CAS: 65332-44-7

Physical Properties

Property code	Value	Unit	Source
gf	361.88	kJ/mol	Joback Method
hf	-175.89	kJ/mol	Joback Method
hfus	37.41	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.605		Crippen Method
mcvol	288.960	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	2057.90		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2057.90		NIST Webbook
rinpol	2036.00		NIST Webbook
tb	726.16	K	Joback Method
tc	921.99	K	Joback Method
tf	343.82	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.84	J/mol×K	726.16	Joback Method

cpg	861.02	J/mol×K	758.80	Joback Method
cpg	880.03	J/mol×K	791.44	Joback Method
cpg	897.88	J/mol×K	824.08	Joback Method
cpg	914.64	J/mol×K	856.71	Joback Method
cpg	930.33	J/mol×K	889.35	Joback Method
cpg	945.00	J/mol×K	921.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65332447&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