

1,2-bis-[2-(Diisopropylamino)ethylthio] ethane

Other names:	Ethane, 1,2-bis[2-(diisopropylamino)ethyl]
Inchi:	InChI=1S/C18H40N2S2/c1-15(2)19(16(3)4)9-11-21-13-14-22-12-10-20(17(5)6)18(7)8/h1
InchiKey:	ZZGOPHQDWOJBGU-UHFFFAOYSA-N
Formula:	C18H40N2S2
SMILES:	CC(C)N(CCSCCSCCN(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]:	348.65

Physical Properties

Property code	Value	Unit	Source
gf	378.72	kJ/mol	Joback Method
hf	-217.17	kJ/mol	Joback Method
hfus	42.59	kJ/mol	Joback Method
hvap	71.83	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.690		Crippen Method
mcvol	317.140	ml/mol	McGowan Method
pc	1202.29	kPa	Joback Method
rinpol	2338.70		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2338.70		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	771.92	K	Joback Method
tc	966.00	K	Joback Method
tf	366.36	K	Joback Method
vc	1.163	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.77	J/mol×K	771.92	Joback Method
cpg	980.18	J/mol×K	804.27	Joback Method
cpg	999.37	J/mol×K	836.61	Joback Method

cpg	1017.39	J/mol×K	868.96	Joback Method
cpg	1034.29	J/mol×K	901.31	Joback Method
cpg	1050.11	J/mol×K	933.65	Joback Method
cpg	1064.89	J/mol×K	966.00	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=R37339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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