

Ethane, 1-[(2-diisopropylamino)ethylthio]-2-[(2-diisopropyl

Other names:

1,9-bis-[Diisopropylamino]-3,4,7-trithianonane

2-Diisopropylaminoethyl 2-(diisopropylaminoethyl)thioethyl disulfide

Inchi:

InChI=1S/C18H40N2S3/c1-15(2)19(16(3)4)9-11-21-13-14-23-22-12-10-20(17(5)6)18(7)8

InchiKey:

SJWQWVJUFZBBOV-UHFFFAOYSA-N

Formula:

C18H40N2S3

SMILES:

CC(C)N(CCSCCSCCN(C(C)C)C(C)C)C(C)C

Mol. weight [g/mol]:

380.72

CAS:

110501-59-2

Physical Properties

Property code	Value	Unit	Source
gf	411.84	kJ/mol	Joback Method
hf	-175.30	kJ/mol	Joback Method
hfus	46.72	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.339		Crippen Method
mvol	333.490	ml/mol	McGowan Method
pc	1216.59	kPa	Joback Method
rinpol	2567.50		NIST Webbook
rinpol	2533.00		NIST Webbook
rinpol	2567.50		NIST Webbook
rinpol	2533.00		NIST Webbook
rinpol	2533.00		NIST Webbook
tb	840.70	K	Joback Method
tc	1048.10	K	Joback Method
tf	400.76	K	Joback Method
vc	1.218	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.61	J/mol×K	840.70	Joback Method
cpg	1047.75	J/mol×K	875.27	Joback Method

cpg	1065.55	J/mol×K	909.83	Joback Method
cpg	1082.04	J/mol×K	944.40	Joback Method
cpg	1097.27	J/mol×K	978.97	Joback Method
cpg	1111.30	J/mol×K	1013.53	Joback Method
cpg	1124.16	J/mol×K	1048.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C110501592&Units=SI

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
hvac:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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