Bis(2-diisopropylaminoethyl) sulfide

Other names: Sulfane, bis(2-diisopropylaminoethyl)-
Inchi: InChI=1S/C16H36N2S/c1-13(2)17(14(3)4)9-11-19-12-10-18(15(5)6)16(7)8/h13-16H,9-12
InchiKey: VRSFIFVYZVUBLG-UHFFFAOYSA-N
Formula: C16H36N2S
SMILES: CC(C)N(CCSCCN(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]: 288.54
CAS: 110501-56-9

Physical Properties

Property code	Value	Unit	Source
gf	328.76	kJ/mol	Joback Method
hf	-217.76	kJ/mol	Joback Method
hfus	33.28	kJ/mol	Joback Method
hvap	60.56	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.957		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1836.10		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1836.10		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	657.38	K	Joback Method
tc	839.15	K	Joback Method
tf	309.42	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.79	J/mol×K	657.38	Joback Method
cpg	789.68	J/mol×K	687.67	Joback Method
cpg	809.50	J/mol×K	717.97	Joback Method

cpg	828.29	J/mol×K	748.26	Joback Method
cpg	846.09	J/mol×K	778.56	Joback Method
cpg	862.94	J/mol×K	808.85	Joback Method
cpg	878.86	J/mol×K	839.15	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=C110501569&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