

Bis(2-diethylaminoethyl) disulfide

Inchi:	InChI=1S/C12H28N2S2/c1-5-13(6-2)9-11-15-16-12-10-14(7-3)8-4/h5-12H2,1-4H3
InchiKey:	MNAQQAGUKWXGLG-UHFFFAOYSA-N
Formula:	C12H28N2S2
SMILES:	CCN(CC)CCSSCCN(CC)CC
Mol. weight [g/mol]:	264.49

Physical Properties

Property code	Value	Unit	Source
gf	337.96	kJ/mol	Joback Method
hf	-72.21	kJ/mol	Joback Method
hfus	41.14	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	3.051		Crippen Method
mcvol	232.600	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	636.40	K	Joback Method
tc	826.94	K	Joback Method
tf	358.74	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.90	J/molxK	636.40	Joback Method
cpg	631.81	J/molxK	668.16	Joback Method
cpg	648.77	J/molxK	699.91	Joback Method
cpg	664.82	J/molxK	731.67	Joback Method

cpg	679.97	J/mol×K	763.42	Joback Method
cpg	694.25	J/mol×K	795.18	Joback Method
cpg	707.71	J/mol×K	826.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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=U226881&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
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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