

bis-(2-Diethylaminoethyl) trisulfide

Inchi:	InChI=1S/C12H28N2S3/c1-5-13(6-2)9-11-15-17-16-12-10-14(7-3)8-4/h5-12H2,1-4H3
InchiKey:	PCNJNSWULFZYJX-UHFFFAOYSA-N
Formula:	C12H28N2S3
SMILES:	CCN(CC)CCSSSCCN(CC)CC
Mol. weight [g/mol]:	296.56

Physical Properties

Property code	Value	Unit	Source
gf	371.08	kJ/mol	Joback Method
hf	-30.34	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	66.84	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.700		Crippen Method
mcvol	248.950	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	705.18	K	Joback Method
tc	910.36	K	Joback Method
tf	393.14	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.45	J/molxK	705.18	Joback Method
cpg	694.85	J/molxK	739.38	Joback Method
cpg	711.16	J/molxK	773.57	Joback Method
cpg	726.44	J/molxK	807.77	Joback Method

cpg	740.69	J/mol×K	841.97	Joback Method
cpg	753.97	J/mol×K	876.16	Joback Method
cpg	766.28	J/mol×K	910.36	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=R334740&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
mvol:	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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