2-Diethylaminoethyl vinyl sulfide

Inchi: InChI=1S/C8H17NS/c1-4-9(5-2)7-8-10-6-3/h6H,3-5,7-8H2,1-2H3
InchiKey: GQAOCNJRHMZKBR-UHFFFAOYSA-N
Formula: C8H17NS
SMILES: C=CSCCN(CC)CC
Mol. weight [g/mol]: 159.29

Physical Properties

Property code	Value	Unit	Source
gf	248.22	kJ/mol	Joback Method
hf	26.38	kJ/mol	Joback Method
hfus	22.35	kJ/mol	Joback Method
hvap	41.59	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	2.205		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1144.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1144.00		NIST Webbook
tb	460.34	K	Joback Method
tc	647.70	K	Joback Method
tf	245.03	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.88	J/mol×K	460.34	Joback Method
cpg	316.10	J/mol×K	491.57	Joback Method
cpg	329.65	J/mol×K	522.79	Joback Method
cpg	342.56	J/mol×K	554.02	Joback Method
cpg	354.83	J/mol×K	585.25	Joback Method
cpg	366.50	J/mol×K	616.48	Joback Method

cpg	377.58	J/mol×K	647.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R334755&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