Methyl 2-diethylaminoethyl sulfide

Inchi: InChI=1S/C7H17NS/c1-4-8(5-2)6-7-9-3/h4-7H2,1-3H3
InchiKey: NCEBDVSAEIMPNE-UHFFFAOYSA-N
Formula: C7H17NS
SMILES: CCN(CC)CCSC
Mol. weight [g/mol]: 147.28

Physical Properties

Property code	Value	Unit	Source
gf	151.96	kJ/mol	Joback Method
hf	-78.41	kJ/mol	Joback Method
hfus	21.04	kJ/mol	Joback Method
hvap	40.04	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.691		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
tb	440.78	K	Joback Method
tc	626.07	K	Joback Method
tf	235.52	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.98	J/mol×K	440.78	Joback Method
cpg	289.77	J/mol×K	471.66	Joback Method
cpg	302.96	J/mol×K	502.54	Joback Method
cpg	315.57	J/mol×K	533.42	Joback Method
cpg	327.61	J/mol×K	564.31	Joback Method
cpg	339.09	J/mol×K	595.19	Joback Method
cpg	350.03	J/mol×K	626.07	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=R338460&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