Methyl 2-diisopropylaminoethyl sulfide

Inchi: InChI=1S/C9H21NS/c1-8(2)10(9(3)4)6-7-11-5/h8-9H,6-7H2,1-5H3
InchiKey: LTZXYLOWXWDULT-UHFFFAOYSA-N
Formula: C9H21NS
SMILES: CSCCN(C(C)C)C(C)C
Mol. weight [g/mol]: 175.34

Physical Properties

Property code	Value	Unit	Source
gf	163.92	kJ/mol	Joback Method
hf	-130.25	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	43.71	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.468		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	1196.00		NIST Webbook
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tb	485.66	K	Joback Method
tc	675.38	K	Joback Method
tf	228.06	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.11	J/mol×K	485.66	Joback Method
cpg	380.61	J/mol×K	517.28	Joback Method
cpg	396.34	J/mol×K	548.90	Joback Method
cpg	411.33	J/mol×K	580.52	Joback Method
cpg	425.60	J/mol×K	612.14	Joback Method
cpg	439.16	J/mol×K	643.76	Joback Method
cpg	452.04	J/mol×K	675.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R338475&Units=SI
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

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