Isopropyl 2-diisopropylaminoethyl sulfide

Inchi: InChI=1S/C11H25NS/c1-9(2)12(10(3)4)7-8-13-11(5)6/h9-11H,7-8H2,1-6H3
InchiKey: ATHRUUFDAYVGPI-UHFFFAOYSA-N
Formula: C11H25NS
SMILES: CC(C)SCCN(C(C)C)C(C)C
Mol. weight [g/mol]: 203.39

Physical Properties

Property code	Value	Unit	Source
gf	178.32	kJ/mol	Joback Method
hf	-176.81	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	47.78	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.247		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1321.00		NIST Webbook
tb	530.98	K	Joback Method
tc	720.24	K	Joback Method
tf	235.60	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.96	J/mol×K	530.98	Joback Method
cpg	478.31	J/mol×K	562.52	Joback Method
cpg	495.78	J/mol×K	594.07	Joback Method
cpg	512.40	J/mol×K	625.61	Joback Method
cpg	528.19	J/mol×K	657.15	Joback Method
cpg	543.18	J/mol×K	688.70	Joback Method
cpg	557.39	J/mol×K	720.24	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=R338455&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