2-Diisopropylaminoethyl ethyl sulfide

Other names: Ethyl 2-diisopropylaminoethyl sulfide
Inchi: InChI=1S/C10H23NS/c1-6-12-8-7-11(9(2)3)10(4)5/h9-10H,6-8H2,1-5H3
InchiKey: JQECUITYJBGTCT-UHFFFAOYSA-N
Formula: C10H23NS
SMILES: CCSCCN(C(C)C)C(C)C
Mol. weight [g/mol]: 189.36
CAS: 110501-54-7

Physical Properties

Property code	Value	Unit	Source
gf	172.34	kJ/mol	Joback Method
hf	-150.89	kJ/mol	Joback Method
hfus	21.76	kJ/mol	Joback Method
hvap	45.94	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.858		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1264.00		NIST Webbook
rinpol	1277.60		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1277.60		NIST Webbook
tb	508.54	K	Joback Method
tc	696.11	K	Joback Method
tf	239.33	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.02	J/mol×K	508.54	Joback Method
cpg	428.28	J/mol×K	539.80	Joback Method

cpg	444.74	J/mol×K	571.06	Joback Method
cpg	460.42	J/mol×K	602.32	Joback Method
cpg	475.34	J/mol×K	633.59	Joback Method
cpg	489.53	J/mol×K	664.85	Joback Method
cpg	502.99	J/mol×K	696.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110501547&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