[2-(Diisopropylamino)ethyl]-(2-mercaptoethyl) sulfide

Other names: 2-(2-Diisopropylamino-ethylsulfanyl)-ethanethiol
Inchi: InChI=1S/C10H23NS2/c1-9(2)11(10(3)4)5-7-13-8-6-12/h9-10,12H,5-8H2,1-4H3
InchiKey: BVWKCXBNLROVOD-UHFFFAOYSA-N
Formula: C10H23NS2
SMILES: CC(C)N(CCSCCS)C(C)C
Mol. weight [g/mol]: 221.43
CAS: 168885-96-9

Physical Properties

Property code	Value	Unit	Source
gf	201.73	kJ/mol	Joback Method
hf	-112.41	kJ/mol	Joback Method
hfus	25.80	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.768		Crippen Method
mcvol	194.440	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
tb	571.40	K	Joback Method
tc	777.28	K	Joback Method
tf	275.79	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.13	J/mol×K	571.40	Joback Method
cpg	486.52	J/mol×K	605.71	Joback Method
cpg	502.97	J/mol×K	640.03	Joback Method
cpg	518.51	J/mol×K	674.34	Joback Method
cpg	533.17	J/mol×K	708.66	Joback Method
cpg	546.98	J/mol×K	742.97	Joback Method
cpg	559.96	J/mol×K	777.28	Joback Method

Sources

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=C168885969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume