S-Propyl-N,N-diisopropyldithiocarbamate

Inchi: InChI=1S/C10H21NS2/c1-6-7-13-10(12)11(8(2)3)9(4)5/h8-9H,6-7H2,1-5H3
InchiKey: LXQUMCXOBIGJCG-UHFFFAOYSA-N
Formula: C10H21NS2
SMILES: CCCSC(=S)N(C(C)C)C(C)C
Mol. weight [g/mol]: 219.41

Physical Properties

Property code	Value	Unit	Source
gf	289.40	kJ/mol	Joback Method
hf	-4.39	kJ/mol	Joback Method
hfus	26.36	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.533		Crippen Method
mcvol	190.140	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1617.00		NIST Webbook
tb	578.58	K	Joback Method
tc	789.02	K	Joback Method
tf	273.60	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.99	J/mol×K	578.58	Joback Method
cpg	469.23	J/mol×K	613.65	Joback Method
cpg	484.49	J/mol×K	648.73	Joback Method
cpg	498.82	J/mol×K	683.80	Joback Method
cpg	512.29	J/mol×K	718.88	Joback Method
cpg	524.94	J/mol×K	753.95	Joback Method
cpg	536.85	J/mol×K	789.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R122255&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