S-Ethyl-N,N-diisopropyldithiocarbamate

Inchi: InChI=1S/C9H19NS2/c1-6-12-9(11)10(7(2)3)8(4)5/h7-8H,6H2,1-5H3
InchiKey: GYWHIYKCCVKRAS-UHFFFAOYSA-N
Formula: C9H19NS2
SMILES: CCSC(=S)N(C(C)C)C(C)C
Mol. weight [g/mol]: 205.38

Physical Properties

Property code	Value	Unit	Source
gf	280.98	kJ/mol	Joback Method
hf	16.25	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	50.44	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.143		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1540.00		NIST Webbook
tb	555.70	K	Joback Method
tc	769.66	K	Joback Method
tf	262.33	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.71	J/mol×K	555.70	Joback Method
cpg	420.31	J/mol×K	591.36	Joback Method
cpg	434.95	J/mol×K	627.02	Joback Method
cpg	448.68	J/mol×K	662.68	Joback Method
cpg	461.55	J/mol×K	698.34	Joback Method
cpg	473.62	J/mol×K	734.00	Joback Method
cpg	484.96	J/mol×K	769.66	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=R122200&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume