S-Isopropyl-N,N-diethyldithiocarbamate

Inchi: InChI=1S/C8H17NS2/c1-5-9(6-2)8(10)11-7(3)4/h7H,5-6H2,1-4H3
InchiKey: AIFGNPOVOGXDOJ-UHFFFAOYSA-N
Formula: C8H17NS2
SMILES: CCN(CC)C(=S)SC(C)C
Mol. weight [g/mol]: 191.36

Physical Properties

Property code	Value	Unit	Source
gf	275.00	kJ/mol	Joback Method
hf	42.17	kJ/mol	Joback Method
hfus	24.71	kJ/mol	Joback Method
hvap	48.60	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.755		Crippen Method
mcvol	161.960	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	1461.00		NIST Webbook
tb	533.26	K	Joback Method
tc	746.10	K	Joback Method
tf	266.06	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.79	J/mol×K	533.26	Joback Method
cpg	372.26	J/mol×K	568.73	Joback Method
cpg	385.83	J/mol×K	604.21	Joback Method
cpg	398.55	J/mol×K	639.68	Joback Method
cpg	410.48	J/mol×K	675.16	Joback Method
cpg	421.67	J/mol×K	710.63	Joback Method
cpg	432.17	J/mol×K	746.10	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=R122235&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