S-(2-Methylallyl)-N,N-dimethyldithiocarbamate

Inchi: InChI=1S/C9H17NS2/c1-5-10(6-2)9(11)12-7-8(3)4/h3,5-7H2,1-2,4H3
InchiKey: NWZQNOBXSVYLDR-UHFFFAOYSA-N
Formula: C9H17NS2
SMILES: C=C(C)CSC(=S)N(CC)CC
Mol. weight [g/mol]: 203.37

Physical Properties

Property code	Value	Unit	Source
gf	365.15	kJ/mol	Joback Method
hf	142.45	kJ/mol	Joback Method
hfus	28.23	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.922		Crippen Method
mcvol	171.750	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	553.14	K	Joback Method
tc	766.25	K	Joback Method
tf	276.61	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.23	J/mol×K	553.14	Joback Method
cpg	398.65	J/mol×K	588.66	Joback Method
cpg	412.15	J/mol×K	624.18	Joback Method
cpg	424.79	J/mol×K	659.69	Joback Method
cpg	436.63	J/mol×K	695.21	Joback Method
cpg	447.73	J/mol×K	730.73	Joback Method
cpg	458.16	J/mol×K	766.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R122151&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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