S-tert-Butyl-N,N-diethyldithiocarbamate

Inchi: InChI=1S/C9H19NS2/c1-6-10(7-2)8(11)12-9(3,4)5/h6-7H2,1-5H3
InchiKey: QKUPZECCOOWFNO-UHFFFAOYSA-N
Formula: C9H19NS2
SMILES: CCN(CC)C(=S)SC(C)(C)C
Mol. weight [g/mol]: 205.38

Physical Properties

Property code	Value	Unit	Source
gf	288.70	kJ/mol	Joback Method
hf	18.06	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	49.92	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.145		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1499.00		NIST Webbook
rinpol	1499.00		NIST Webbook
tb	553.35	K	Joback Method
tc	771.20	K	Joback Method
tf	294.75	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.32	J/mol×K	553.35	Joback Method
cpg	423.14	J/mol×K	589.66	Joback Method
cpg	437.86	J/mol×K	625.97	Joback Method
cpg	451.55	J/mol×K	662.27	Joback Method
cpg	464.30	J/mol×K	698.58	Joback Method
cpg	476.19	J/mol×K	734.89	Joback Method
cpg	487.30	J/mol×K	771.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R122275&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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