S-Allyl-N,N-diethyldithiocarbamate

Inchi: InChI=1S/C8H15NS2/c1-4-7-11-8(10)9(5-2)6-3/h4H,1,5-7H2,2-3H3
InchiKey: NLZGRCKPBHBOGE-UHFFFAOYSA-N
Formula: C8H15NS2
SMILES: C=CCSC(=S)N(CC)CC
Mol. weight [g/mol]: 189.34

Physical Properties

Property code	Value	Unit	Source
gf	365.28	kJ/mol	Joback Method
hf	172.88	kJ/mol	Joback Method
hfus	26.95	kJ/mol	Joback Method
hvap	48.32	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.532		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	1516.00		NIST Webbook
tb	530.38	K	Joback Method
tc	743.07	K	Joback Method
tf	279.30	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.63	J/mol×K	530.38	Joback Method
cpg	352.05	J/mol×K	565.83	Joback Method
cpg	364.60	J/mol×K	601.28	Joback Method
cpg	376.33	J/mol×K	636.73	Joback Method
cpg	387.29	J/mol×K	672.18	Joback Method
cpg	397.56	J/mol×K	707.62	Joback Method
cpg	407.18	J/mol×K	743.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R122166&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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