Allyl dimethyldithiocarbamate

Other names: S-Allyl-N,N-dimethyldithiocarbamate
Carbamic acid, dimethyldithio-, allyl ester
Allyl N,N-dimethyldithiocarbamate
Inchi: InChI=1S/C6H11NS2/c1-4-5-9-6(8)7(2)3/h4H,1,5H2,2-3H3
InchiKey: ZFMLVJCASVPGIT-UHFFFAOYSA-N
Formula: C6H11NS2
SMILES: C=CCSC(=S)N(C)C
Mol. weight [g/mol]: 161.29
CAS: 20821-66-3

Physical Properties

Property code	Value	Unit	Source
gf	348.44	kJ/mol	Joback Method
hf	214.16	kJ/mol	Joback Method
hfus	21.77	kJ/mol	Joback Method
hvap	43.87	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.752		Crippen Method
mcvol	129.480	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
rinpol	1417.00		NIST Webbook
tb	484.62	K	Joback Method
tc	704.32	K	Joback Method
tf	256.76	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.50	J/mol×K	484.62	Joback Method
cpg	263.99	J/mol×K	521.24	Joback Method
cpg	274.67	J/mol×K	557.85	Joback Method
cpg	284.57	J/mol×K	594.47	Joback Method
cpg	293.77	J/mol×K	631.09	Joback Method

cpg	302.33	J/mol×K	667.70	Joback Method
cpg	310.29	J/mol×K	704.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20821663&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

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