Carbamodithioic acid, dibutyl-, propyl ester

Other names:	Carbamic acid, dibutyldithio-, propyl ester
	S-Propyl N,N-di-n-butyldithiocarbamate
Inchi:	InChI=1S/C12H25NS2/c1-4-7-9-13(10-8-5-2)12(14)15-11-6-3/h4-11H2,1-3H3
InchiKey:	UFDGCMYVJSFYQM-UHFFFAOYSA-N
Formula:	C12H25NS2
SMILES:	CCCCN(CCCC)C(=S)SCCC
Mol. weight [g/mol]:	247.46
CAS:	19047-84-8

Physical Properties

Property code	Value	Unit	Source
gf	311.12	kJ/mol	Joback Method
hf	-35.11	kJ/mol	Joback Method
hfus	38.59	kJ/mol	Joback Method
hvap	57.89	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.317		Crippen Method
mcvol	218.320	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1867.00		NIST Webbook
tb	625.22	K	Joback Method
tc	821.76	K	Joback Method
tf	326.14	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.33	J/mol×K	625.22	Joback Method
cpg	569.86	J/mol×K	657.98	Joback Method
cpg	585.47	J/mol×K	690.73	Joback Method
cpg	600.23	J/mol×K	723.49	Joback Method
cpg	614.19	J/mol×K	756.25	Joback Method
cpg	627.39	J/mol×K	789.01	Joback Method

cpg	639.89	J/mol×K	821.76	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=C19047848&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