S-Butyl-N,N-dipropyldithiocarbamate

Inchi: InChI=1S/C11H23NS2/c1-4-7-10-14-11(13)12(8-5-2)9-6-3/h4-10H2,1-3H3
InchiKey: NEGRKPXTVRFKNK-UHFFFAOYSA-N
Formula: C11H23NS2
SMILES: CCCCSC(=S)N(CCC)CCC
Mol. weight [g/mol]: 233.44

Physical Properties

Property code	Value	Unit	Source
gf	302.70	kJ/mol	Joback Method
hf	-14.47	kJ/mol	Joback Method
hfus	36.00	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.927		Crippen Method
mcvol	204.230	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
tb	602.34	K	Joback Method
tc	801.49	K	Joback Method
tf	314.87	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.05	J/mol×K	602.34	Joback Method
cpg	518.09	J/mol×K	635.53	Joback Method
cpg	533.23	J/mol×K	668.72	Joback Method
cpg	547.52	J/mol×K	701.91	Joback Method
cpg	561.01	J/mol×K	735.11	Joback Method
cpg	573.76	J/mol×K	768.30	Joback Method
cpg	585.82	J/mol×K	801.49	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=R122186&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