Dipropyldithiocarbamic acid

Inchi: InChI=1S/C7H15NS2/c1-3-5-8(6-4-2)7(9)10/h3-6H2,1-2H3,(H,9,10)
InchiKey: BQCRLWBELMWYQA-UHFFFAOYSA-N
Formula: C7H15NS2
SMILES: CCCN(CCC)C(=S)S
Mol. weight [g/mol]: 177.33
CAS: 25179-61-7

Physical Properties

Property code	Value	Unit	Source
gf	265.29	kJ/mol	Joback Method
hf	-15.20 ± 3.90	kJ/mol	NIST Webbook
hfus	25.55	kJ/mol	Joback Method
hvap	46.69	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.323		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
tb	504.90	K	Joback Method
tc	716.66	K	Joback Method
tf	271.85	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.60	J/mol×K	504.90	Joback Method
cpg	323.80	J/mol×K	540.19	Joback Method
cpg	336.14	J/mol×K	575.49	Joback Method
cpg	347.68	J/mol×K	610.78	Joback Method
cpg	358.48	J/mol×K	646.08	Joback Method
cpg	368.59	J/mol×K	681.37	Joback Method
cpg	378.09	J/mol×K	716.66	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=C25179617&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume