3,5-Dipropyl-[1,2,4]trithiolane, stereoisomer 2

Inchi: InChI=1S/C8H16S3/c1-3-5-7-9-8(6-4-2)11-10-7/h7-8H,3-6H2,1-2H3
InchiKey: RJVZZGYMVBJRLX-UHFFFAOYSA-N
Formula: C8H16S3
SMILES: CCCC1SSC(CCC)S1
Mol. weight [g/mol]: 208.41

Physical Properties

Property code	Value	Unit	Source
gf	164.90	kJ/mol	Joback Method
hf	-32.53	kJ/mol	Joback Method
hfus	22.45	kJ/mol	Joback Method
hvap	50.79	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.367		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
ripol	1820.00		NIST Webbook
ripol	1820.00		NIST Webbook
tb	536.54	K	Joback Method
tc	771.68	K	Joback Method
tf	436.93	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.49	J/mol×K	536.54	Joback Method
cpg	376.15	J/mol×K	575.73	Joback Method
cpg	391.81	J/mol×K	614.92	Joback Method
cpg	406.49	J/mol×K	654.11	Joback Method
cpg	420.25	J/mol×K	693.30	Joback Method
cpg	433.13	J/mol×K	732.49	Joback Method
cpg	445.17	J/mol×K	771.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R495197&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume