Dipropargyl sulfide

Other names:	3-(2-Propynylsulfanyl)-1-propyne
	4-Thia-1,6-heptadiyne
Inchi:	InChI=1S/C6H6S/c1-3-5-7-6-4-2/h1-2H,5-6H2
InchiKey:	XPTMJJIPRSWBDK-UHFFFAOYSA-N
Formula:	C6H6S
SMILES:	C#CCSCC#C
Mol. weight [g/mol]:	110.18
CAS:	13702-09-5

Physical Properties

Property code	Value	Unit	Source
gf	478.90	kJ/mol	Joback Method
hf	458.50	kJ/mol	Joback Method
hfus	21.38	kJ/mol	Joback Method
hvap	35.48	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	0.986		Crippen Method
mcvol	94.550	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
rinpol	862.00		NIST Webbook
rinpol	862.00		NIST Webbook
tb	385.70	K	Joback Method
tc	604.98	K	Joback Method
tf	285.72	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.46	J/mol×K	385.70	Joback Method
cpg	165.10	J/mol×K	422.25	Joback Method
cpg	172.29	J/mol×K	458.79	Joback Method
cpg	179.06	J/mol×K	495.34	Joback Method
cpg	185.43	J/mol×K	531.89	Joback Method

cpg	191.41	J/mol×K	568.44	Joback Method
cpg	197.02	J/mol×K	604.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13702095&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