

(E,E) Bis(1-propenyl)sulfide

Inchi:	InChI=1S/C6H10S/c1-3-5-7-6-4-2/h3-6H,1-2H3/b5-3+,6-4+
InchiKey:	RJDJXOBGMMKPMH-GGWOSOGESA-N
Formula:	C6H10S
SMILES:	CC=CSC=CC
Mol. weight [g/mol]:	114.21
CAS:	65819-74-1

Physical Properties

Property code	Value	Unit	Source
gf	193.20	kJ/mol	Joback Method
hf	109.14	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hvap	35.68	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.787		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	413.78	K	Joback Method
tc	623.09	K	Joback Method
tf	181.62	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.75	J/molxK	413.78	Joback Method
cpg	186.51	J/molxK	448.66	Joback Method
cpg	196.64	J/molxK	483.55	Joback Method
cpg	206.18	J/molxK	518.43	Joback Method
cpg	215.15	J/molxK	553.32	Joback Method
cpg	223.59	J/molxK	588.20	Joback Method
cpg	231.53	J/molxK	623.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65819741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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