(E) Isopropyl-1-propenylsulfide

Inchi: InChI=1S/C6H12S/c1-4-5-7-6(2)3/h4-6H,1-3H3/b5-4+
InchiKey: IZLJYHRILGAGIM-SNAWJCMRSA-N
Formula: C6H12S
SMILES: CC=CSC(C)C
Mol. weight [g/mol]: 116.22
CAS: 61865-99-4

Physical Properties

Property code	Value	Unit	Source
gf	110.54	kJ/mol	Joback Method
hf	-13.36	kJ/mol	Joback Method
hfus	12.11	kJ/mol	Joback Method
hvap	35.34	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.662		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	409.18	K	Joback Method
tc	612.79	K	Joback Method
tf	171.70	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.23	J/mol×K	409.18	Joback Method
cpg	202.76	J/mol×K	443.11	Joback Method
cpg	213.72	J/mol×K	477.05	Joback Method
cpg	224.15	J/mol×K	510.98	Joback Method
cpg	234.05	J/mol×K	544.92	Joback Method
cpg	243.44	J/mol×K	578.85	Joback Method
cpg	252.35	J/mol×K	612.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61865994&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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