

(E) t-Butyl-1-propenylsulfide

Inchi:	InChI=1S/C7H14S/c1-5-6-8-7(2,3)4/h5-6H,1-4H3/b6-5+
InchiKey:	NXPJZODHTFSBSK-AATRIKPKSA-N
Formula:	C7H14S
SMILES:	CC=CSC(C)(C)C
Mol. weight [g/mol]:	130.25
CAS:	61866-00-0

Physical Properties

Property code	Value	Unit	Source
gf	124.24	kJ/mol	Joback Method
hf	-37.47	kJ/mol	Joback Method
hfus	10.80	kJ/mol	Joback Method
hvap	36.66	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.052		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
tb	429.27	K	Joback Method
tc	639.64	K	Joback Method
tf	200.39	K	Joback Method
vc	0.451	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.26	J/mol×K	429.27	Joback Method
cpg	246.13	J/mol×K	464.33	Joback Method
cpg	259.16	J/mol×K	499.39	Joback Method
cpg	271.39	J/mol×K	534.46	Joback Method
cpg	282.85	J/mol×K	569.52	Joback Method
cpg	293.59	J/mol×K	604.58	Joback Method
cpg	303.66	J/mol×K	639.64	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61866000&Units=SI

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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