

trans-1-(t-Butylthio)-2-butene

Inchi:	InChI=1S/C8H16S/c1-5-6-7-9-8(2,3)4/h5-6H,7H2,1-4H3/b6-5+
InchiKey:	CQTWVLLLOIALFQN-AATRIKPKSA-N
Formula:	C8H16S
SMILES:	CC=CCSC(C)(C)C
Mol. weight [g/mol]:	144.28
CAS:	107183-90-4

Physical Properties

Property code	Value	Unit	Source
gf	132.66	kJ/mol	Joback Method
hf	-58.11	kJ/mol	Joback Method
hfus	13.39	kJ/mol	Joback Method
hvap	38.88	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.094		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	452.15	K	Joback Method
tc	659.90	K	Joback Method
tf	211.66	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.43	J/mol×K	452.15	Joback Method
cpg	288.38	J/mol×K	486.77	Joback Method
cpg	302.45	J/mol×K	521.40	Joback Method
cpg	315.67	J/mol×K	556.02	Joback Method
cpg	328.08	J/mol×K	590.65	Joback Method
cpg	339.75	J/mol×K	625.27	Joback Method
cpg	350.69	J/mol×K	659.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107183904&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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