sec-Butyl isobutyl sulfide

Other names: 2,5-dimethyl-4-thiaheptane
Inchi: InChI=1S/C8H18S/c1-5-8(4)9-6-7(2)3/h7-8H,5-6H2,1-4H3
InchiKey: ZXOHSPNYEDQIBI-UHFFFAOYSA-N
Formula: C8H18S
SMILES: CCC(C)SCC(C)C
Mol. weight [g/mol]: 146.29
CAS: 16900-02-0

Physical Properties

Property code	Value	Unit	Source
gf	44.72	kJ/mol	Joback Method
hf	-177.14	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	39.44	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	3.174		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	991.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	991.00		NIST Webbook
tb	450.34	K	Joback Method
tc	644.50	K	Joback Method
tf	184.32	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.13	J/mol×K	450.34	Joback Method
cpg	301.81	J/mol×K	482.70	Joback Method
cpg	315.88	J/mol×K	515.06	Joback Method
cpg	329.34	J/mol×K	547.42	Joback Method

cpg	342.19	J/mol×K	579.78	Joback Method
cpg	354.46	J/mol×K	612.14	Joback Method
cpg	366.15	J/mol×K	644.50	Joback Method

Sources

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=C16900020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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