Butyl isobutyl sulfide

Other names: 2-methyl-4-thiaoctane
Inchi: InChI=1S/C8H18S/c1-4-5-6-9-7-8(2)3/h8H,4-7H2,1-3H3
InchiKey: PWXRDOSRCIGJDM-UHFFFAOYSA-N
Formula: C8H18S
SMILES: CCCCSCC(C)C
Mol. weight [g/mol]: 146.29
CAS: 1741-85-1

Physical Properties

Property code	Value	Unit	Source
gf	47.16	kJ/mol	Joback Method
hf	-171.86	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	39.83	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.176		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook
tb	450.78	K	Joback Method
tc	640.58	K	Joback Method
tf	199.32	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.04	J/mol×K	450.78	Joback Method
cpg	301.31	J/mol×K	482.41	Joback Method
cpg	315.00	J/mol×K	514.05	Joback Method
cpg	328.11	J/mol×K	545.68	Joback Method
cpg	340.66	J/mol×K	577.31	Joback Method

cpg	352.65	J/mol×K	608.94	Joback Method
cpg	364.09	J/mol×K	640.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1741851&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume