Octane, 1-(butylthio)-

Other names:	5-Thiatridecane
	Butyl octyl sulfide
	Sulfide, butyl octyl
Inchi:	InChI=1S/C12H26S/c1-3-5-7-8-9-10-12-13-11-6-4-2/h3-12H2,1-2H3
InchiKey:	UNIAPWPIAGJFDG-UHFFFAOYSA-N
Formula:	C12H26S
SMILES:	CCCCCCCCSCCCC
Mol. weight [g/mol]:	202.40
CAS:	16900-07-5

Physical Properties

Property code	Value	Unit	Source
gf	83.28	kJ/mol	Joback Method
hf	-249.14	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.880		Crippen Method
mcvol	196.290	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
ripol	1684.00		NIST Webbook
tb	542.74	K	Joback Method
tc	721.16	K	Joback Method
tf	259.40	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	472.53	J/mol×K	542.74	Joback Method
cpg	489.74	J/mol×K	572.48	Joback Method
cpg	506.22	J/mol×K	602.21	Joback Method
cpg	521.99	J/mol×K	631.95	Joback Method
cpg	537.07	J/mol×K	661.69	Joback Method
cpg	551.47	J/mol×K	691.42	Joback Method
cpg	565.21	J/mol×K	721.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59133e+01
Coeff. B	-4.90231e+03
Coeff. C	-8.96740e+01
Temperature range (K), min.	403.41
Temperature range (K), max.	552.08

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16900075&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume