

Octane, 1-(propylthio)-

Other names:	4-Thiadodecane Octyl propyl sulfide Sulfide, octyl propyl
Inchi:	InChI=1S/C11H24S/c1-3-5-6-7-8-9-11-12-10-4-2/h3-11H2,1-2H3
InchiKey:	GPJXDRJGQAKGLH-UHFFFAOYSA-N
Formula:	C11H24S
SMILES:	CCCCCCCCSCCC
Mol. weight [g/mol]:	188.37
CAS:	3698-93-9

Physical Properties

Property code	Value	Unit	Source
gf	74.86	kJ/mol	Joback Method
hf	-228.50	kJ/mol	Joback Method
hfus	28.38	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.490		Crippen Method
mcvol	182.200	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1382.00		NIST Webbook
rinpol	1382.00		NIST Webbook
ripol	1592.00		NIST Webbook
tb	519.86	K	Joback Method
tc	700.00	K	Joback Method
tf	248.13	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.34	J/molxK	519.86	Joback Method
cpg	439.87	J/molxK	549.88	Joback Method
cpg	455.71	J/molxK	579.91	Joback Method

cpg	470.88	J/mol×K	609.93	Joback Method
cpg	485.39	J/mol×K	639.95	Joback Method
cpg	499.25	J/mol×K	669.98	Joback Method
cpg	512.48	J/mol×K	700.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60036e+01
Coeff. B	-4.79775e+03
Coeff. C	-8.51710e+01
Temperature range (K), min.	390.45
Temperature range (K), max.	533.89

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3698939&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/ci9903071
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

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