

# Tetradecyl methanesulfonate

<b>Inchi:</b>	InChI=1S/C15H32O3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-19(2,16)17/h3-15H2,1-2H1
<b>InchiKey:</b>	SHHTUKUQKILIDO-UHFFFAOYSA-N
<b>Formula:</b>	C15H32O3S
<b>SMILES:</b>	CCCCCCCCCCCCCOS(C)(=O)=O
<b>Mol. weight [g/mol]:</b>	292.48
<b>CAS:</b>	6222-16-8

## Physical Properties

Property code	Value	Unit	Source
gf	-498.12	kJ/mol	Joback Method
hf	-938.50	kJ/mol	Joback Method
hfus	47.17	kJ/mol	Joback Method
hvap	70.03	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.664		Crippen Method
mcvol	256.170	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
tb	612.80	K	Joback Method
tc	771.87	K	Joback Method
tf	319.60	K	Joback Method
vc	1.020	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.61	J/molxK	612.80	Joback Method
cpg	703.81	J/molxK	639.31	Joback Method
cpg	721.28	J/molxK	665.82	Joback Method
cpg	738.02	J/molxK	692.34	Joback Method
cpg	754.03	J/molxK	718.85	Joback Method
cpg	769.33	J/molxK	745.36	Joback Method
cpg	783.92	J/molxK	771.87	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6222168&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6222168&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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