

1-Hexadecanesulfonyl chloride

Other names:	Hexadecylsulfonyl chloride n-Hexadecane sulfonyl chloride Sulfonyl chloride, 1-hexadecane- 1-Hexadecanesulphonyl chloride hexadecane-1-sulphonyl chloride
Inchi:	InChI=1S/C16H33ClO2S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20(17,18)19/h2-16H2
InchiKey:	YOSVFFVBSPQTTP-UHFFFAOYSA-N
Formula:	C16H33ClO2S
SMILES:	CCCCCCCCCCCCCCCCS(=O)(=O)Cl
Mol. weight [g/mol]:	324.95
CAS:	38775-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-396.63	kJ/mol	Joback Method
hf	-842.66	kJ/mol	Joback Method
hfus	52.77	kJ/mol	Joback Method
hvap	74.23	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	6.036		Crippen Method
mcvol	276.630	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
tb	650.69	K	Joback Method
tc	814.51	K	Joback Method
tf	338.56	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.42	J/mol×K	650.69	Joback Method
cpg	765.57	J/mol×K	677.99	Joback Method
cpg	782.91	J/mol×K	705.30	Joback Method
cpg	799.45	J/mol×K	732.60	Joback Method

cpg	815.20	J/mol×K	759.90	Joback Method
cpg	830.19	J/mol×K	787.20	Joback Method
cpg	844.41	J/mol×K	814.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38775381&Units=SI
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

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
hvp:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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