

Disulfide, dihexyl

Other names:	Hexyl disulfide Dihexyl disulfide di-n-Hexyl disulfide n-Hexyl disulfide dihexyl disulphide
Inchi:	InChI=1S/C12H26S2/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3-12H2,1-2H3
InchiKey:	GJPDBURPGLWRPW-UHFFFAOYSA-N
Formula:	C12H26S2
SMILES:	CCCCCSCCCCCC
Mol. weight [g/mol]:	234.47
CAS:	10496-15-8

Physical Properties

Property code	Value	Unit	Source
gf	116.40	kJ/mol	Joback Method
hf	-207.27	kJ/mol	Joback Method
hfus	35.10	kJ/mol	Joback Method
hvap	55.94	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.528		Crippen Method
mcvol	212.640	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
ripol	1927.00		NIST Webbook
ripol	1927.00		NIST Webbook
tb	611.52	K	Joback Method
tc	806.24	K	Joback Method
tf	293.80	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.12	J/molxK	611.52	Joback Method
cpg	553.45	J/molxK	643.97	Joback Method

cpg	569.95	J/mol×K	676.43	Joback Method
cpg	585.61	J/mol×K	708.88	Joback Method
cpg	600.46	J/mol×K	741.33	Joback Method
cpg	614.51	J/mol×K	773.79	Joback Method
cpg	627.78	J/mol×K	806.24	Joback Method
hvapt	64.90	kJ/mol	518.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10496158&Units=SI
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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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