

4,7,10,16,19,22-Hexaoxa-1,13-dithiacyclotetracosane

Inchi:	InChI=1S/C16H32O6S2/c1-5-19-9-13-23-15-11-21-7-3-18-4-8-22-12-16-24-14-10-20-6-2
InchiKey:	VBWOPQXSPKWFGU-UHFFFAOYSA-N
Formula:	C16H32O6S2
SMILES:	C1COCCSCCOCCOCCOCCSCCOCCO1
Mol. weight [g/mol]:	384.55
CAS:	297-13-2

Physical Properties

Property code	Value	Unit	Source
gf	-538.80	kJ/mol	Joback Method
hf	-1111.27	kJ/mol	Joback Method
hfus	45.35	kJ/mol	Joback Method
hvap	93.73	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	1.566		Crippen Method
mcvol	293.360	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
tb	923.92	K	Joback Method
tc	1233.11	K	Joback Method
tf	544.66	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.18	J/molxK	923.92	Joback Method
cpg	1018.43	J/molxK	975.45	Joback Method
cpg	1030.61	J/molxK	1026.98	Joback Method
cpg	1036.43	J/molxK	1078.52	Joback Method
cpg	1035.59	J/molxK	1130.05	Joback Method
cpg	1027.80	J/molxK	1181.58	Joback Method
cpg	1012.78	J/molxK	1233.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C297132&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/23-312-9/4-7-10-16-19-22-Hexaoxa-1-13-dithiacyclotetracosane.pdf>

Generated by Cheméo on 2024-04-25 19:48:29.143122294 +0000 UTC m=+16363758.063699688.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.