

4,7,13,16-Tetraoxa-1,10-dithiacyclooctadecane-1,10-dithione

Inchi: InChI=1S/C28H44O10S4/c1-25-5-9-27(10-6-25)41(29,30)37-39(3)21-17-33-13-15-35-19
InchiKey: DZSCWYJYKXSIIH-UHFFFAOYSA-N
Formula: C28H44O10S4
SMILES: Cc1ccc(S(=O)(=O)OS2(C)CCOCCOCCS(C)(OS(=O)(=O)c3ccc(C)cc3)CCOCCOCC2)cc1
Mol. weight [g/mol]: 668.90

Physical Properties

Property code	Value	Unit	Source
gf	-1343.96	kJ/mol	Joback Method
hf	-2002.25	kJ/mol	Joback Method
hfus	78.78	kJ/mol	Joback Method
hvap	158.94	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.193		Crippen Method
mcvol	479.700	ml/mol	McGowan Method
pc	1388.15	kPa	Joback Method
tb	1325.48	K	Joback Method
tc	1624.07	K	Joback Method
tf	781.86	K	Joback Method
vc	1.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1466.90	J/molxK	1325.48	Joback Method
cpg	1404.14	J/molxK	1375.25	Joback Method
cpg	1328.34	J/molxK	1425.01	Joback Method
cpg	1238.98	J/molxK	1474.78	Joback Method
cpg	1135.55	J/molxK	1524.54	Joback Method
cpg	1017.56	J/molxK	1574.31	Joback Method
cpg	884.50	J/molxK	1624.07	Joback Method

Sources

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=B6002152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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