Propargite

Other names:	Sulfurous acid, 2-[4-(1,1-dimethylethyl)phenoxy]cyclohexyl 2-propynyl ester
	Sulfurous acid, 2-(p-tert-butylphenoxy)cyclohexyl 2-propynyl ester
	Comite
	Cyclosulfyne
	D 014
	Naugatuck D 014
	Omite
	Omite 57E
	Omite 85E
	Propargil
	2-(p-tert-Butylphenoxy)cyclohexyl 2'-propynyl sulfite
	2-(p-tert-Butylphenoxy)cyclohexyl propargyl sulfite
	2-(p-tert-Butylphenoxy)cyclohexyl 2-propynyl sulfite
	2-(Para-tert-butylphenoxy)cyclohexyl-2'-propynyl sulfite
	BPPS
	Propargite, isomer 2
	Propargite, isomer 1
Inchi:	InChI=1S/C19H26O4S/c1-5-14-21-24(20)23-18-9-7-6-8-17(18)22-16-12-10-15(11-13-16)
InchiKey:	ZYHMJXZULPZUED-UHFFFAOYSA-N
Formula:	C19H26O4S
SMILES:	C#CCOS(=O)OC1CCCCC1Oc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	350.47
CAS:	2312-35-8

Physical Properties

Property code	Value	Unit	Source
gf	-78.18	kJ/mol	Joback Method
hf	-495.70	kJ/mol	Joback Method
hfus	38.40	kJ/mol	Joback Method
hvap	79.46	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.919		Crippen Method
mcvol	275.180	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	2403.00		NIST Webbook
rinpol	2398.00		NIST Webbook
rinpol	2402.00		NIST Webbook

ripol	3342.00		NIST Webbook
tb	793.09	K	Joback Method
tc	1025.00	K	Joback Method
tf	498.53	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.36	J/mol×K	793.09	Joback Method
cpg	851.92	J/mol×K	831.74	Joback Method
cpg	869.71	J/mol×K	870.39	Joback Method
cpg	885.78	J/mol×K	909.04	Joback Method
cpg	900.15	J/mol×K	947.69	Joback Method
cpg	912.83	J/mol×K	986.34	Joback Method
cpg	923.87	J/mol×K	1025.00	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2312358&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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume