((1,2-Diethylethylene)bis(p-phenylene))diacetate

Other names: Hexestrol, O,O'-di(acetyl)-
Inchi: InChI=1S/C22H26O4/c1-5-21(17-7-11-19(12-8-17)25-15(3)23)22(6-2)18-9-13-20(14-10-1
InchiKey: GWEREDCWIUZACS-UHFFFAOYSA-N
Formula: C22H26O4
SMILES: CCC(c1ccc(OC(C)=O)cc1)C(CC)c1ccc(OC(C)=O)cc1
Mol. weight [g/mol]: 354.44
CAS: 4547-76-6

Physical Properties

Property code	Value	Unit	Source
gf	-132.80	kJ/mol	Joback Method
hf	-547.45	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	87.98	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.225		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	917.78	K	Joback Method
tc	1144.86	K	Joback Method
tf	529.90	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.76	J/mol×K	917.78	Joback Method
cpg	912.19	J/mol×K	955.63	Joback Method
cpg	925.21	J/mol×K	993.47	Joback Method
cpg	936.84	J/mol×K	1031.32	Joback Method
cpg	947.14	J/mol×K	1069.17	Joback Method
cpg	956.14	J/mol×K	1107.01	Joback Method

cpg	963.87	J/mol×K	1144.86	Joback Method
dvisc	0.0004479	Pa×s	529.90	Joback Method
dvisc	0.0002343	Pa×s	594.55	Joback Method
dvisc	0.0001391	Pa×s	659.19	Joback Method
dvisc	0.0000907	Pa×s	723.84	Joback Method
dvisc	0.0000634	Pa×s	788.49	Joback Method
dvisc	0.0000468	Pa×s	853.13	Joback Method
dvisc	0.0000361	Pa×s	917.78	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4547766&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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