1-(4-Tert-butylphenyl) 2-phenyl phthalate

Inchi: InChI=1S/C24H22O4/c1-24(2,3)17-13-15-19(16-14-17)28-23(26)21-12-8-7-11-20(21)22(
InchiKey: VDWFGIANGMAWOH-UHFFFAOYSA-N
Formula: C24H22O4
SMILES: CC(C)(C)c1ccc(OC(=O)c2ccccc2C(=O)Oc2ccccc2)cc1
Mol. weight [g/mol]: 374.43
CAS: 116595-14-3

Physical Properties

Property code	Value	Unit	Source
gf	4.17	kJ/mol	Joback Method
hf	-350.39	kJ/mol	Joback Method
hfus	37.42	kJ/mol	Joback Method
hvap	94.19	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.422		Crippen Method
mcvol	292.620	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
tb	987.87	K	Joback Method
tc	1241.75	K	Joback Method
tf	611.28	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.66	J/mol×K	987.87	Joback Method
cpg	921.04	J/mol×K	1030.18	Joback Method
cpg	932.01	J/mol×K	1072.50	Joback Method
cpg	941.68	J/mol×K	1114.81	Joback Method
cpg	950.15	J/mol×K	1157.12	Joback Method
cpg	957.54	J/mol×K	1199.43	Joback Method
cpg	963.95	J/mol×K	1241.75	Joback Method
dvisc	0.0002329	Pa×s	611.28	Joback Method
dvisc	0.0001357	Pa×s	674.04	Joback Method

dvisc	0.0000867	Pa×s	736.81	Joback Method
dvisc	0.0000594	Pa×s	799.57	Joback Method
dvisc	0.0000430	Pa×s	862.34	Joback Method
dvisc	0.0000326	Pa×s	925.10	Joback Method
dvisc	0.0000255	Pa×s	987.87	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=C116595143&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume