Bis-(3-benzoxyphenyl) phthalate

Inchi: InChI=1S/C34H26O6/c35-33(39-29-17-9-15-27(21-29)37-23-25-11-3-1-4-12-25)31-19-7-
InchiKey: PIWMKMLXJKXBBF-UHFFFAOYSA-N
Formula: C34H26O6
SMILES: O=C(Oc1cccc(OCc2ccccc2)c1)c1ccccc1C(=O)Oc1cccc(OCc2ccccc2)c1
Mol. weight [g/mol]: 530.57
CAS: 116402-24-5

Physical Properties

Property code	Value	Unit	Source
gf	90.72	kJ/mol	Joback Method
hf	-350.89	kJ/mol	Joback Method
hfus	60.80	kJ/mol	Joback Method
hvap	127.78	kJ/mol	Joback Method
log10ws	-10.10		Crippen Method
logp	7.283		Crippen Method
mcvol	397.740	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
tb	1323.08	K	Joback Method
tc	1619.91	K	Joback Method
tf	831.38	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.39	J/mol×K	1323.08	Joback Method
cpg	1282.82	J/mol×K	1372.55	Joback Method
cpg	1280.09	J/mol×K	1422.02	Joback Method
cpg	1275.37	J/mol×K	1471.50	Joback Method
cpg	1268.80	J/mol×K	1520.97	Joback Method
cpg	1260.53	J/mol×K	1570.44	Joback Method
cpg	1250.73	J/mol×K	1619.91	Joback Method
dvisc	0.0000337	Pa×s	831.38	Joback Method
dvisc	0.0000207	Pa×s	913.33	Joback Method

dvisc	0.0000138	Pa×s	995.28	Joback Method
dvisc	0.0000098	Pa×s	1077.23	Joback Method
dvisc	0.0000073	Pa×s	1159.18	Joback Method
dvisc	0.0000056	Pa×s	1241.13	Joback Method
dvisc	0.0000045	Pa×s	1323.08	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=C116402245&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