Terephthalic acid, di(2-phenoxyethyl) ester

Inchi: InChI=1S/C24H22O6/c25-23(29-17-15-27-21-7-3-1-4-8-21)19-11-13-20(14-12-19)24(26)30-18-16-28-22-9-5-2-6-10-22/h1-14H,15-18H2

InchiKey: JJTLCMPVLZYLPH-UHFFFAOYSA-N

Formula: C24H22O6

SMILES: O=C(OCCOc1ccccc1)c1ccc(C(=O)OCCOc2ccccc2)cc1

Mol. weight [g/mol]: 406.43

Physical Properties

Property code	Value	Unit	Source
gf	-199.04	kJ/mol	Joback Method
hf	-594.61	kJ/mol	Joback Method
hfus	47.60	kJ/mol	Joback Method
hvap	99.64	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.158		Crippen Method
mcvol	304.360	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	2524.00		NIST Webbook
rinpol	2524.00		NIST Webbook
tb	1030.96	K	Joback Method
tc	1275.31	K	Joback Method
tf	640.80	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.41	J/mol×K	1030.96	Joback Method
cpg	989.49	J/mol×K	1234.59	Joback Method
cpg	986.93	J/mol×K	1193.86	Joback Method
cpg	982.67	J/mol×K	1153.14	Joback Method
cpg	976.69	J/mol×K	1112.41	Joback Method
cpg	968.95	J/mol×K	1071.69	Joback Method
cpg	990.41	J/mol×K	1275.31	Joback Method
dvisc	0.0000180	Pa×s	1030.96	Joback Method

dvisc	0.0000228	Pa×s	965.93	Joback Method
dvisc	0.0000299	Pa×s	900.91	Joback Method
dvisc	0.0000408	Pa×s	835.88	Joback Method
dvisc	0.0000586	Pa×s	770.85	Joback Method
dvisc	0.0000901	Pa×s	705.83	Joback Method
dvisc	0.0001513	Pa×s	640.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416049&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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