Terephthalic acid, isobutyl 2-phenoxyethyl ester

Inchi: InChI=1S/C20H22O5/c1-15(2)14-25-20(22)17-10-8-16(9-11-17)19(21)24-13-12-23-18-6-

InchiKey: VOEUMMADTBFQPI-UHFFFAOYSA-N

Formula: C20H22O5

SMILES: CC(C)COC(=O)c1ccc(C(=O)OCCOc2ccccc2)cc1

Mol. weight [g/mol]: 342.39

Physical Properties

Property code	Value	Unit	Source
gf	-242.57	kJ/mol	Joback Method
hf	-621.64	kJ/mol	Joback Method
hfus	38.49	kJ/mol	Joback Method
hvap	85.66	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.735		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	889.90	K	Joback Method
tc	1115.53	K	Joback Method
tf	532.07	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.26	J/mol×K	889.90	Joback Method
cpg	863.42	J/mol×K	1077.93	Joback Method
cpg	855.32	J/mol×K	1040.32	Joback Method
cpg	845.87	J/mol×K	1002.72	Joback Method
cpg	835.06	J/mol×K	965.11	Joback Method
cpg	822.86	J/mol×K	927.51	Joback Method
cpg	870.21	J/mol×K	1115.53	Joback Method
dvisc	0.0000385	Pa×s	889.90	Joback Method

dvisc	0.0000495	Pa×s	830.26	Joback Method
dvisc	0.0000661	Pa×s	770.62	Joback Method
dvisc	0.0000927	Pa×s	710.99	Joback Method
dvisc	0.0001383	Pa×s	651.35	Joback Method
dvisc	0.0002237	Pa×s	591.71	Joback Method
dvisc	0.0004028	Pa×s	532.07	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=U416042&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