Terephthalic acid, 3-methoxyphenyl octyl ester

Inchi: InChI=1S/C23H28O5/c1-3-4-5-6-7-8-16-27-22(24)18-12-14-19(15-13-18)23(25)28-21-11

InchiKey: MOJUGCLRWVRIKF-UHFFFAOYSA-N

Formula: C23H28O5

SMILES: CCCCCCCCOC(=O)c1ccc(C(=O)Oc2cccc(OC)c2)cc1

Mol. weight [g/mol]: 384.47

Physical Properties

Property code	Value	Unit	Source
gf	-224.50	kJ/mol	Joback Method
hf	-689.75	kJ/mol	Joback Method
hfus	49.39	kJ/mol	Joback Method
hvap	93.39	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.432		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinpol	3264.00		NIST Webbook
rinpol	3264.00		NIST Webbook
tb	963.96	K	Joback Method
tc	1187.86	K	Joback Method
tf	593.40	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.39	J/mol×K	963.96	Joback Method
cpg	996.76	J/mol×K	1001.28	Joback Method
cpg	1008.63	J/mol×K	1038.59	Joback Method
cpg	1019.01	J/mol×K	1075.91	Joback Method
cpg	1027.94	J/mol×K	1113.23	Joback Method
cpg	1035.43	J/mol×K	1150.55	Joback Method
cpg	1041.52	J/mol×K	1187.86	Joback Method
dvisc	0.0002370	Pa×s	593.40	Joback Method

dvisc	0.0001403	Pa×s	655.16	Joback Method
dvisc	0.0000909	Pa×s	716.92	Joback Method
dvisc	0.0000631	Pa×s	778.68	Joback Method
dvisc	0.0000462	Pa×s	840.44	Joback Method
dvisc	0.0000353	Pa×s	902.20	Joback Method
dvisc	0.0000280	Pa×s	963.96	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=U415824&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