Terephthalic acid, hexyl 3-methoxyphenyl ester

Inchi: InChI=1S/C21H24O5/c1-3-4-5-6-14-25-20(22)16-10-12-17(13-11-16)21(23)26-19-9-7-8-1

InchiKey: LCDCHSQJXMYTHP-UHFFFAOYSA-N

Formula: C21H24O5

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

Mol. weight [g/mol]: 356.41

Physical Properties

Property code	Value	Unit	Source
gf	-241.34	kJ/mol	Joback Method
hf	-648.47	kJ/mol	Joback Method
hfus	44.21	kJ/mol	Joback Method
hvap	88.94	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.652		Crippen Method
mcvol	279.980	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	3091.00		NIST Webbook
rinpol	3091.00		NIST Webbook
tb	918.20	K	Joback Method
tc	1141.23	K	Joback Method
tf	570.86	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.55	J/mol×K	918.20	Joback Method
cpg	878.94	J/mol×K	955.37	Joback Method
cpg	890.91	J/mol×K	992.54	Joback Method
cpg	901.49	J/mol×K	1029.71	Joback Method
cpg	910.68	J/mol×K	1066.88	Joback Method
cpg	918.51	J/mol×K	1104.05	Joback Method
cpg	925.00	J/mol×K	1141.23	Joback Method
dvisc	0.0002929	Pa×s	570.86	Joback Method

dvisc	0.0001774	Pa×s	628.75	Joback Method
dvisc	0.0001169	Pa×s	686.64	Joback Method
dvisc	0.0000822	Pa×s	744.53	Joback Method
dvisc	0.0000608	Pa×s	802.42	Joback Method
dvisc	0.0000468	Pa×s	860.31	Joback Method
dvisc	0.0000373	Pa×s	918.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415822&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

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