Isophthalic acid, heptyl 4-methoxyphenyl ester

Inchi: InChI=1S/C22H26O5/c1-3-4-5-6-7-15-26-21(23)17-9-8-10-18(16-17)22(24)27-20-13-11-1
InchiKey: ZLUDARUCILIWIA-UHFFFAOYSA-N
Formula: C22H26O5
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(OC)cc2)c1
Mol. weight [g/mol]: 370.44

Physical Properties

Property code	Value	Unit	Source
gf	-232.92	kJ/mol	Joback Method
hf	-669.11	kJ/mol	Joback Method
hfus	46.80	kJ/mol	Joback Method
hvap	91.16	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.042		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1453.46	kPa	Joback Method
rinpol	3095.00		NIST Webbook
rinpol	3095.00		NIST Webbook
tb	941.08	K	Joback Method
tc	1164.13	K	Joback Method
tf	582.13	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.20	J/mol×K	941.08	Joback Method
cpg	937.58	J/mol×K	978.26	Joback Method
cpg	949.51	J/mol×K	1015.43	Joback Method
cpg	960.00	J/mol×K	1052.61	Joback Method
cpg	969.08	J/mol×K	1089.78	Joback Method
cpg	976.76	J/mol×K	1126.96	Joback Method
cpg	983.08	J/mol×K	1164.13	Joback Method
dvisc	0.0002639	Pa×s	582.13	Joback Method

dvisc	0.0001580	Pa×s	641.95	Joback Method
dvisc	0.0001032	Pa×s	701.78	Joback Method
dvisc	0.0000721	Pa×s	761.61	Joback Method
dvisc	0.0000531	Pa×s	821.43	Joback Method
dvisc	0.0000407	Pa×s	881.25	Joback Method
dvisc	0.0000323	Pa×s	941.08	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=U344481&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