Isophthalic acid, heptyl 3-methylphenyl ester

Inchi: InChI=1S/C22H26O4/c1-3-4-5-6-7-14-25-21(23)18-11-9-12-19(16-18)22(24)26-20-13-8-1
InchiKey: AXRJMLIKGOEVHY-UHFFFAOYSA-N
Formula: C22H26O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2cccc(C)c2)c1
Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-127.92	kJ/mol	Joback Method
hf	-536.89	kJ/mol	Joback Method
hfus	45.61	kJ/mol	Joback Method
hvap	88.75	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.341		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2886.00		NIST Webbook
rinpol	2886.00		NIST Webbook
tb	918.66	K	Joback Method
tc	1141.14	K	Joback Method
tf	559.90	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.78	J/mol×K	918.66	Joback Method
cpg	911.00	J/mol×K	955.74	Joback Method
cpg	923.89	J/mol×K	992.82	Joback Method
cpg	935.48	J/mol×K	1029.90	Joback Method
cpg	945.81	J/mol×K	1066.98	Joback Method
cpg	954.92	J/mol×K	1104.06	Joback Method
cpg	962.84	J/mol×K	1141.14	Joback Method
dvisc	0.0003717	Pa×s	559.90	Joback Method

dvisc	0.0002185	Pa×s	619.69	Joback Method
dvisc	0.0001410	Pa×s	679.49	Joback Method
dvisc	0.0000977	Pa×s	739.28	Joback Method
dvisc	0.0000715	Pa×s	799.07	Joback Method
dvisc	0.0000547	Pa×s	858.87	Joback Method
dvisc	0.0000433	Pa×s	918.66	Joback Method

Sources

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=U344520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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