Isophthalic acid, 2-methylbutyl pentyl ester

Inchi: InChI=1S/C18H26O4/c1-4-6-7-11-21-17(19)15-9-8-10-16(12-15)18(20)22-13-14(3)5-2/h8
InchiKey: FFIHZVQVEBSFEP-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CCCCCOC(=O)c1cccc(C(=O)OCC(C)CC)c1
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-266.82	kJ/mol	Joback Method
hf	-684.67	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.237		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook
tb	795.04	K	Joback Method
tc	997.07	K	Joback Method
tf	460.88	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.78	J/mol×K	795.04	Joback Method
cpg	777.64	J/mol×K	828.71	Joback Method
cpg	792.42	J/mol×K	862.38	Joback Method
cpg	806.14	J/mol×K	896.06	Joback Method
cpg	818.82	J/mol×K	929.73	Joback Method
cpg	830.46	J/mol×K	963.40	Joback Method
cpg	841.10	J/mol×K	997.07	Joback Method
dvisc	0.0008214	Pa×s	460.88	Joback Method

dvisc	0.0004305	Pa×s	516.57	Joback Method
dvisc	0.0002558	Pa×s	572.27	Joback Method
dvisc	0.0001668	Pa×s	627.96	Joback Method
dvisc	0.0001165	Pa×s	683.65	Joback Method
dvisc	0.0000860	Pa×s	739.35	Joback Method
dvisc	0.0000662	Pa×s	795.04	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=U344731&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