Isophthalic acid, 2-methylcyclohexyl pentyl ester

Inchi: InChI=1S/C20H28O4/c1-3-4-7-13-23-19(21)16-10-8-11-17(14-16)20(22)24-18-12-6-5-9-1

InchiKey: ZWXJMXYJDIQDMA-UHFFFAOYSA-N

Formula: C20H28O4

SMILES: CCCCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-230.80	kJ/mol	Joback Method
hf	-686.69	kJ/mol	Joback Method
hfus	39.69	kJ/mol	Joback Method
hvap	81.48	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.769		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	2557.00		NIST Webbook
rinpol	2557.00		NIST Webbook
tb	856.12	K	Joback Method
tc	1075.16	K	Joback Method
tf	501.56	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.81	J/mol×K	856.12	Joback Method
cpg	948.40	J/mol×K	1038.65	Joback Method
cpg	937.07	J/mol×K	1002.15	Joback Method
cpg	924.26	J/mol×K	965.64	Joback Method
cpg	909.97	J/mol×K	929.13	Joback Method
cpg	894.16	J/mol×K	892.63	Joback Method
cpg	958.29	J/mol×K	1075.16	Joback Method
dvisc	0.0000735	Pa×s	856.12	Joback Method

dvisc	0.0000936	Pa×s	797.03	Joback Method
dvisc	0.0001239	Pa×s	737.93	Joback Method
dvisc	0.0001721	Pa×s	678.84	Joback Method
dvisc	0.0002547	Pa×s	619.75	Joback Method
dvisc	0.0004093	Pa×s	560.65	Joback Method
dvisc	0.0007355	Pa×s	501.56	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=U345749&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