1,3-benzenedicarboxylic acid, dihexyl ester

Other names: 1,3-Benzenedicarboxylic acid, dihexyl ester
Inchi: InChI=1S/C20H30O4/c1-3-5-7-9-14-23-19(21)17-12-11-13-18(16-17)20(22)24-15-10-8-6
InchiKey: FGWAPOKSKMNBEN-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCCCCCC)c1
Mol. weight [g/mol]: 334.45
CAS: 4623-71-6

Physical Properties

Property code	Value	Unit	Source
af	1.0205		Cheméo Relay (1.0)
hf	-841.91	kJ/mol	Cheméo Relay (1.0)
hfus	46.78	kJ/mol	Joback Method
hvap	92.84	kJ/mol	Cheméo Relay (1.0)
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-6.03		Cheméo Relay (1.0)
logp	5.161		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
tb	636.12	K	Cheméo Relay (1.0)
tc	832.38	K	Cheméo Relay (1.0)
tf	291.50	K	Cheméo Relay (1.0)
vc	1.076	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.72	J/mol×K	841.24	Joback Method
cpg	893.85	J/mol×K	874.57	Joback Method
cpg	908.85	J/mol×K	907.91	Joback Method
cpg	922.75	J/mol×K	941.24	Joback Method
cpg	935.56	J/mol×K	974.58	Joback Method
cpg	947.32	J/mol×K	1007.91	Joback Method
cpg	958.03	J/mol×K	1041.25	Joback Method

dvisc	0.0005930	Pa×s	498.42	Joback Method
dvisc	0.0003251	Pa×s	555.56	Joback Method
dvisc	0.0001994	Pa×s	612.69	Joback Method
dvisc	0.0001329	Pa×s	669.83	Joback Method
dvisc	0.0000945	Pa×s	726.97	Joback Method
dvisc	0.0000705	Pa×s	784.10	Joback Method
dvisc	0.0000548	Pa×s	841.24	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4623716&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume