1,4-Benzenedicarboxylic acid, dihexyl ester

Other names: Terephthalic acid, dihexyl ester
Terephthalate, dihexyl
Dihexyl terephthalate
Inchi: InChI=1S/C20H30O4/c1-3-5-7-9-15-23-19(21)17-11-13-18(14-12-17)20(22)24-16-10-8-6
InchiKey: MLIPQTRXLNTCRS-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCCCCCOC(=O)c1ccc(C(=O)OCCCCCC)cc1
Mol. weight [g/mol]: 334.45
CAS: 1818-96-8

Physical Properties

Property code	Value	Unit	Source
gf	-247.54	kJ/mol	Joback Method
hf	-720.67	kJ/mol	Joback Method
hfus	46.78	kJ/mol	Joback Method
hvap	81.36	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.161		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2463.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2463.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	841.24	K	Joback Method
tc	1041.25	K	Joback Method
tf	498.42	K	Joback Method
vc	1.095	m3/kmol	Joback Method

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1818968&Units=SI
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

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