Dipropyl isophthalate

Other names: 1,3-benzenedicarboxylic acid, dipropyl ester
Inchi: InChI=1S/C14H18O4/c1-3-8-17-13(15)11-6-5-7-12(10-11)14(16)18-9-4-2/h5-7,10H,3-4,8
InchiKey: FZNKCFJDFGDMKU-UHFFFAOYSA-N
Formula: C14H18O4
SMILES: CCCOC(=O)c1cccc(C(=O)OCCC)c1
Mol. weight [g/mol]: 250.29
CAS: 3143-06-4

Physical Properties

Property code	Value	Unit	Source
gf	-298.06	kJ/mol	Joback Method
hf	-596.83	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	68.01	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.820		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1829.00		NIST Webbook
tb	703.96	K	Joback Method
tc	909.90	K	Joback Method
tf	430.80	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.98	J/mol×K	703.96	Joback Method
cpg	554.36	J/mol×K	738.28	Joback Method
cpg	567.84	J/mol×K	772.61	Joback Method

cpg	580.44	J/mol×K	806.93	Joback Method
cpg	592.16	J/mol×K	841.25	Joback Method
cpg	603.00	J/mol×K	875.58	Joback Method
cpg	612.97	J/mol×K	909.90	Joback Method
dvisc	0.0009874	Pa×s	430.80	Joback Method
dvisc	0.0005866	Pa×s	476.33	Joback Method
dvisc	0.0003816	Pa×s	521.85	Joback Method
dvisc	0.0002660	Pa×s	567.38	Joback Method
dvisc	0.0001956	Pa×s	612.91	Joback Method
dvisc	0.0001501	Pa×s	658.43	Joback Method
dvisc	0.0001192	Pa×s	703.96	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3143064&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

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