1,4-Benzenedicarboxylic acid, dioctyl ester

Other names: dioctyl terephthalate
Inchi: InChI=1S/C24H38O4/c1-3-5-7-9-11-13-19-27-23(25)21-15-17-22(18-16-21)24(26)28-20-
InchiKey: OEIWPNWSDYFMIL-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CCCCCCCCOC(=O)c1ccc(C(=O)OCCCCCCCC)cc1
Mol. weight [g/mol]: 390.56
CAS: 4654-26-6

Physical Properties

Property code	Value	Unit	Source
gf	-213.86	kJ/mol	Joback Method
hf	-803.23	kJ/mol	Joback Method
hfus	57.14	kJ/mol	Joback Method
hvap	90.27	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	6.721		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	2860.00		NIST Webbook
rinpol	2860.00		NIST Webbook
tb	932.76	K	Joback Method
tc	1142.45	K	Joback Method
tf	543.50	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.44	J/mol×K	932.76	Joback Method
cpg	1191.30	J/mol×K	1107.50	Joback Method
cpg	1179.51	J/mol×K	1072.55	Joback Method
cpg	1166.46	J/mol×K	1037.60	Joback Method
cpg	1152.13	J/mol×K	1002.66	Joback Method
cpg	1136.46	J/mol×K	967.71	Joback Method

cpg	1201.88	J/mol×K	1142.45	Joback Method
dvisc	0.0000308	Pa×s	932.76	Joback Method
dvisc	0.0000401	Pa×s	867.88	Joback Method
dvisc	0.0000544	Pa×s	803.01	Joback Method
dvisc	0.0000780	Pa×s	738.13	Joback Method
dvisc	0.0001199	Pa×s	673.25	Joback Method
dvisc	0.0002018	Pa×s	608.38	Joback Method
dvisc	0.0003848	Pa×s	543.50	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4654266&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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