BIS(3,5,5-TRIMETHYLHEXYL) PHTHALATE

Other names: 1,2-Benzenedicarboxylic acid, bis(3,5,5-trimethylhexyl) ester
Inchi: InChI=1S/C26H42O4/c1-19(17-25(3,4)5)13-15-29-23(27)21-11-9-10-12-22(21)24(28)30-
InchiKey: GDJOUZYAIHWDCA-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CC(CCOC(=O)c1ccccc1C(=O)OCCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 418.62

Physical Properties

Property code	Value	Unit	Source
hf	-1004.29	kJ/mol	Cheméo Relay (1.0)
hfus	40.45	kJ/mol	Joback Method
hvap	100.44	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.34		Cheméo Relay (1.0)
logp	6.925		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	945.58	kPa	Joback Method
tb	665.79	K	Cheméo Relay (1.0)
tf	323.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.27	J/mol×K	971.18	Joback Method
cpg	1261.82	J/mol×K	1007.85	Joback Method
cpg	1278.03	J/mol×K	1044.53	Joback Method
cpg	1292.99	J/mol×K	1081.20	Joback Method
cpg	1306.81	J/mol×K	1117.88	Joback Method
cpg	1319.57	J/mol×K	1154.55	Joback Method
cpg	1331.37	J/mol×K	1191.23	Joback Method
dvisc	0.0002973	Pa×s	540.88	Joback Method
dvisc	0.0001242	Pa×s	612.60	Joback Method
dvisc	0.0000623	Pa×s	684.31	Joback Method
dvisc	0.0000356	Pa×s	756.03	Joback Method
dvisc	0.0000224	Pa×s	827.75	Joback Method

dvisc	0.0000152	Pa×s	899.46	Joback Method
dvisc	0.0000109	Pa×s	971.18	Joback Method
hvapt	113.60	kJ/mol	363.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14103618&Units=SI

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):

Legend

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
hvapt: Enthalpy of vaporization at a given temperature
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
tf: Normal melting (fusion) point