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]: 418.61
CAS: 14103-61-8

Physical Properties

Property code	Value	Unit	Source
gf	-196.22	kJ/mol	Joback Method
hf	-872.57	kJ/mol	Joback Method
hfus	40.45	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.925		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	945.58	kPa	Joback Method
tb	971.18	K	Joback Method
tc	1191.23	K	Joback Method
tf	540.88	K	Joback Method
vc	1.397	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14103618&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume