1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester

Other names: Bis(2-ethylhexyl) isophthalate
Di-2-ethylhexyl isophthalate
Dioctyl isophthalate
DOIP
Isophthalic acid, bis(2-ethylhexyl) ester
Bis-(2-ethylhexyl)ester kyseliny isoftalove
Flexol plasticizer 380
Isophthalic acid, di(2-ethylhexyl) ester
Bis-(2-ethylhexyl) isophahalate
1,3-Benzenedicarboxylic acid, 1,3-bis(2-ethylhexyl) ester
NSC 6358

Inchi: InChI=1S/C24H38O4/c1-5-9-12-19(7-3)17-27-23(25)21-14-11-15-22(16-21)24(26)28-18-

InchiKey: WXZOXVVKILCOPG-UHFFFAOYSA-N

Formula: C24H38O4

SMILES: CCCCC(CC)COC(=O)c1cccc(C(=O)OCC(CC)CCCC)c1

Mol. weight [g/mol]: 390.56

CAS: 137-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-218.74	kJ/mol	Joback Method
hf	-813.79	kJ/mol	Joback Method
hfus	50.10	kJ/mol	Joback Method
hvap	89.49	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.433		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1041.93	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	931.88	K	Joback Method
tc	1142.43	K	Joback Method
tf	513.50	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.29	J/mol×K	931.88	Joback Method
cpg	1137.32	J/mol×K	966.97	Joback Method
cpg	1152.94	J/mol×K	1002.06	Joback Method
cpg	1167.20	J/mol×K	1037.16	Joback Method
cpg	1180.14	J/mol×K	1072.25	Joback Method
cpg	1191.79	J/mol×K	1107.34	Joback Method
cpg	1202.19	J/mol×K	1142.43	Joback Method
dvisc	0.0004856	Pa×s	513.50	Joback Method
dvisc	0.0002219	Pa×s	583.23	Joback Method
dvisc	0.0001198	Pa×s	652.96	Joback Method
dvisc	0.0000729	Pa×s	722.69	Joback Method
dvisc	0.0000484	Pa×s	792.42	Joback Method
dvisc	0.0000343	Pa×s	862.15	Joback Method
dvisc	0.0000256	Pa×s	931.88	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=C137893&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