1,2-Benzenedicarboxylic acid, bis(6-methylheptyl) ester

Other names: 27554-26-3
Bis(6-methylheptyl) phthalate
Diisooctyl phthalate
Phthalic acid, bis(6-methylheptyl) ester

Inchi: InChI=1S/C24H38O4/c1-19(2)13-7-5-11-17-27-23(25)21-15-9-10-16-22(21)24(26)28-18-

InchiKey: IJFPVINAQGWBRJ-UHFFFAOYSA-N

Formula: C24H38O4

SMILES: CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCCCCCC(C)C

Mol. weight [g/mol]: 390.56

CAS: 131-20-4

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	-6.64		Estimated Solubility Method
log10ws	-6.64		Aqueous Solubility Prediction Method
logp	6.433		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1041.93	kPa	Joback Method
rinpol	2525.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2540.00		NIST Webbook
rinpol	2540.00		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	1202.19	J/mol×K	1142.43	Joback Method
cpg	1191.79	J/mol×K	1107.34	Joback Method
cpg	1180.14	J/mol×K	1072.25	Joback Method
cpg	1167.20	J/mol×K	1037.16	Joback Method
cpg	1152.94	J/mol×K	1002.06	Joback Method
cpg	1137.32	J/mol×K	966.97	Joback Method
cpg	1120.29	J/mol×K	931.88	Joback Method
dvisc	0.0004856	Pa×s	513.50	Joback Method
dvisc	0.0000256	Pa×s	931.88	Joback Method
dvisc	0.0000343	Pa×s	862.15	Joback Method
dvisc	0.0000484	Pa×s	792.42	Joback Method
dvisc	0.0000729	Pa×s	722.69	Joback Method
dvisc	0.0001198	Pa×s	652.96	Joback Method
dvisc	0.0002219	Pa×s	583.23	Joback Method
hvapt	92.40	kJ/mol	436.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52850e+01
Coeff. B	-6.40227e+03
Coeff. C	-1.08683e+02
Temperature range (K), min.	535.57
Temperature range (K), max.	750.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.53737e+02
Coeff. B	-2.01401e+04
Coeff. C	-1.86055e+01
Coeff. D	3.42367e-06

Temperature range (K), min.	260.00
Temperature range (K), max.	851.00

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C131204&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1162
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume