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

Other names: Diisoamyl phthalate
Diisopentyl phthalate
Phthalic acid, diisopentyl ester
Disoamyl phthalate
Phthalic acid, di(3-methylbutyl) ester

Inchi: InChI=1S/C18H26O4/c1-13(2)9-11-21-17(19)15-7-5-6-8-16(15)18(20)22-12-10-14(3)4/h5

InchiKey: JANBFCARANRIKJ-UHFFFAOYSA-N

Formula: C18H26O4

SMILES: CC(C)CCOC(=O)c1ccccc1C(=O)OCCC(C)C

Mol. weight [g/mol]: 306.40

CAS: 605-50-5

Physical Properties

Property code	Value	Unit	Source
chs	-9857.90 ± 5.00	kJ/mol	NIST Webbook
gf	-269.26	kJ/mol	Joback Method
hf	-689.95	kJ/mol	Joback Method
hfs	-941.00 ± 5.00	kJ/mol	NIST Webbook
hfus	34.56	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.092		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	794.60	K	Joback Method
tc	999.14	K	Joback Method
tf	445.88	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	842.26	J/mol×K	999.14	Joback Method
cpg	831.61	J/mol×K	965.05	Joback Method
cpg	819.91	J/mol×K	930.96	Joback Method
cpg	807.15	J/mol×K	896.87	Joback Method
cpg	793.31	J/mol×K	862.78	Joback Method
cpg	778.37	J/mol×K	828.69	Joback Method
cpg	762.32	J/mol×K	794.60	Joback Method
dvisc	0.0009566	Pa×s	445.88	Joback Method
dvisc	0.0000608	Pa×s	794.60	Joback Method
dvisc	0.0000803	Pa×s	736.48	Joback Method
dvisc	0.0001112	Pa×s	678.36	Joback Method
dvisc	0.0001637	Pa×s	620.24	Joback Method
dvisc	0.0002611	Pa×s	562.12	Joback Method
dvisc	0.0004637	Pa×s	504.00	Joback Method
hvapt	81.60	kJ/mol	500.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C605505&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume