Phthalic acid, di(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

Physical Properties

Property code	Value	Unit	Source
af	0.8575		Cheméo Relay (1.0)
chs	-9857.90 ± 5.00	kJ/mol	NIST Webbook
hf	-802.37	kJ/mol	Cheméo Relay (1.0)
hfs	-941.00 ± 5.00	kJ/mol	NIST Webbook
hfus	34.56	kJ/mol	Joback Method
hvap	85.43	kJ/mol	Cheméo Relay (1.0)
ie	9.20	eV	Cheméo Relay (1.0)
log10ws	-4.98		Cheméo Relay (1.0)
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	612.85	K	Cheméo Relay (1.0)
tc	809.39	K	Cheméo Relay (1.0)
tf	252.63	K	Cheméo Relay (1.0)
vc	0.948	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

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

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C605505&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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

ie: Ionization energy

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

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