

Terephthalic acid, isobutyl 5-methylhex-2-yl ester

Inchi:	InChI=1S/C19H28O4/c1-13(2)6-7-15(5)23-19(21)17-10-8-16(9-11-17)18(20)22-12-14(3)-
InchiKey:	PTKLRIVZBHLNNW-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CC(C)CCC(C)OC(=O)c1ccc(C(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-263.28	kJ/mol	Joback Method
hf	-715.87	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	77.97	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.481		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinqol	2534.00		NIST Webbook
tb	817.04	K	Joback Method
tc	1023.15	K	Joback Method
tf	442.15	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.65	J/molxK	817.04	Joback Method
cpg	837.06	J/molxK	851.39	Joback Method
cpg	852.29	J/molxK	885.74	Joback Method
cpg	866.34	J/molxK	920.09	Joback Method
cpg	879.25	J/molxK	954.45	Joback Method
cpg	891.04	J/molxK	988.80	Joback Method
cpg	901.72	J/molxK	1023.15	Joback Method
dvisc	0.0010191	Paxs	442.15	Joback Method
dvisc	0.0004484	Paxs	504.63	Joback Method

dvisc	0.0002364	Paxs	567.11	Joback Method
dvisc	0.0001415	Paxs	629.60	Joback Method
dvisc	0.0000930	Paxs	692.08	Joback Method
dvisc	0.0000655	Paxs	754.56	Joback Method
dvisc	0.0000486	Paxs	817.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382996&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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