Terephthalic acid, isohexyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C19H28O4/c1-13(2)7-6-12-22-18(20)16-8-10-17(11-9-16)19(21)23-15(5)14(3)4

InchiKey: VWKWGNHIXSUFSX-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CC(C)CCCOC(=O)c1ccc(C(=O)OC(C)C(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
rinpol	2234.00		NIST Webbook
tb	817.04	K	Joback Method
tc	1023.15	K	Joback Method
tf	442.15	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002364	Pa×s	567.11	Joback Method
dvisc	0.0001415	Pa×s	629.60	Joback Method
dvisc	0.0000930	Pa×s	692.08	Joback Method
dvisc	0.0000655	Pa×s	754.56	Joback Method
dvisc	0.0000486	Pa×s	817.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356273&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

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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