Phthalic acid, 2,4-dimethylpent-3-yl isobutyl ester

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

InchiKey: UMDZJHHFHULWIG-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-265.72	kJ/mol	Joback Method
hf	-721.15	kJ/mol	Joback Method
hfus	30.10	kJ/mol	Joback Method
hvap	77.59	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.337		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	816.60	K	Joback Method
tc	1025.20	K	Joback Method
tf	427.15	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.17	J/mol×K	816.60	Joback Method
cpg	892.13	J/mol×K	990.43	Joback Method
cpg	880.31	J/mol×K	955.67	Joback Method
cpg	867.32	J/mol×K	920.90	Joback Method
cpg	853.16	J/mol×K	886.13	Joback Method
cpg	837.78	J/mol×K	851.37	Joback Method
cpg	902.81	J/mol×K	1025.20	Joback Method
dvisc	0.0000446	Pa×s	816.60	Joback Method

dvisc	0.0000611	Pa×s	751.69	Joback Method
dvisc	0.0000888	Pa×s	686.78	Joback Method
dvisc	0.0001394	Pa×s	621.88	Joback Method
dvisc	0.0002432	Pa×s	556.97	Joback Method
dvisc	0.0004913	Pa×s	492.06	Joback Method
dvisc	0.0012291	Pa×s	427.15	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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