

Phthalic acid, 3,3-dimethylbut-2-yl isobutyl ester

Inchi:	InChI=1S/C18H26O4/c1-12(2)11-21-16(19)14-9-7-8-10-15(14)17(20)22-13(3)18(4,5)6/h7
InchiKey:	FYVGFDNOHPOTNO-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CC(C)COC(=O)c1ccccc1C(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-266.42	kJ/mol	Joback Method
hf	-698.70	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Joback Method
hvap	74.84	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.091		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1981.00		NIST Webbook
tb	791.37	K	Joback Method
tc	1003.75	K	Joback Method
tf	448.30	K	Joback Method
vc	0.961	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.90	J/molxK	791.37	Joback Method
cpg	780.27	J/molxK	826.77	Joback Method
cpg	795.45	J/molxK	862.16	Joback Method
cpg	809.48	J/molxK	897.56	Joback Method
cpg	822.41	J/molxK	932.96	Joback Method
cpg	834.26	J/molxK	968.35	Joback Method
cpg	845.08	J/molxK	1003.75	Joback Method
dvisc	0.0009271	Paxs	448.30	Joback Method
dvisc	0.0004305	Paxs	505.48	Joback Method

dvisc	0.0002336	Paxs	562.66	Joback Method
dvisc	0.0001419	Paxs	619.84	Joback Method
dvisc	0.0000938	Paxs	677.01	Joback Method
dvisc	0.0000661	Paxs	734.19	Joback Method
dvisc	0.0000490	Paxs	791.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357001&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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