isobutyl hydrogen phthalate

Other names: 2-(Isobutoxycarbonyl)benzoic acid
Inchi: InChI=1S/C12H14O4/c1-8(2)7-16-12(15)10-6-4-3-5-9(10)11(13)14/h3-6,8H,7H2,1-2H3,(H
InchiKey: RZJSUWQGFCHNFS-UHFFFAOYSA-N
Formula: C12H14O4
SMILES: CC(C)COC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 222.24
CAS: 30833-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-349.16	kJ/mol	Joback Method
hf	-580.84	kJ/mol	Joback Method
hfus	25.44	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.198		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	727.52	K	Joback Method
tc	932.19	K	Joback Method
tf	431.85	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.22	J/mol×K	727.52	Joback Method
cpg	474.41	J/mol×K	761.63	Joback Method
cpg	484.85	J/mol×K	795.74	Joback Method
cpg	494.55	J/mol×K	829.86	Joback Method
cpg	503.54	J/mol×K	863.97	Joback Method
cpg	511.83	J/mol×K	898.08	Joback Method

cpg	519.44	J/mol×K	932.19	Joback Method
dvisc	0.0013756	Pa×s	431.85	Joback Method
dvisc	0.0005593	Pa×s	481.13	Joback Method
dvisc	0.0002688	Pa×s	530.41	Joback Method
dvisc	0.0001463	Pa×s	579.68	Joback Method
dvisc	0.0000876	Pa×s	628.96	Joback Method
dvisc	0.0000565	Pa×s	678.24	Joback Method
dvisc	0.0000387	Pa×s	727.52	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=C30833535&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

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