

Isophthalic acid, isobutyl neopentyl ester

Inchi:	InChI=1S/C17H24O4/c1-12(2)10-20-15(18)13-7-6-8-14(9-13)16(19)21-11-17(3,4)5/h6-9,
InchiKey:	BDHFEBLVTOXLIJ-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-272.40	kJ/mol	Joback Method
hf	-672.78	kJ/mol	Joback Method
hfus	28.07	kJ/mol	Joback Method
hvap	73.00	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.702		Crippen Method
mvol	241.510	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	768.93	K	Joback Method
tc	980.32	K	Joback Method
tf	452.03	K	Joback Method
vc	0.910	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.75	J/molxK	768.93	Joback Method
cpg	722.71	J/molxK	804.16	Joback Method
cpg	737.54	J/molxK	839.39	Joback Method
cpg	751.28	J/molxK	874.62	Joback Method
cpg	763.96	J/molxK	909.85	Joback Method
cpg	775.62	J/molxK	945.08	Joback Method
cpg	786.30	J/molxK	980.32	Joback Method
dvisc	0.0008716	Paxs	452.03	Joback Method

dvisc	0.0004446	Paxs	504.85	Joback Method
dvisc	0.0002576	Paxs	557.66	Joback Method
dvisc	0.0001641	Paxs	610.48	Joback Method
dvisc	0.0001123	Paxs	663.30	Joback Method
dvisc	0.0000813	Paxs	716.11	Joback Method
dvisc	0.0000615	Paxs	768.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343860&Units=SI

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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