

Isophthalic acid, isobutyl 3-methylpentyl ester

Inchi:	InChI=1S/C18H26O4/c1-5-14(4)9-10-21-17(19)15-7-6-8-16(11-15)18(20)22-12-13(2)3/h6
InchiKey:	XMZJOEFWSIHUMF-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCC(C)CCOC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-269.26	kJ/mol	Joback Method
hf	-689.95	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.092		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	794.60	K	Joback Method
tc	999.14	K	Joback Method
tf	445.88	K	Joback Method
vc	0.972	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.32	J/molxK	794.60	Joback Method
cpg	778.37	J/molxK	828.69	Joback Method
cpg	793.31	J/molxK	862.78	Joback Method
cpg	807.15	J/molxK	896.87	Joback Method
cpg	819.91	J/molxK	930.96	Joback Method
cpg	831.61	J/molxK	965.05	Joback Method
cpg	842.26	J/molxK	999.14	Joback Method
dvisc	0.0009566	Paxs	445.88	Joback Method

dvisc	0.0004637	Paxs	504.00	Joback Method
dvisc	0.0002611	Paxs	562.12	Joback Method
dvisc	0.0001637	Paxs	620.24	Joback Method
dvisc	0.0001112	Paxs	678.36	Joback Method
dvisc	0.0000803	Paxs	736.48	Joback Method
dvisc	0.0000608	Paxs	794.60	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=U356540&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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