

Isophthalic acid, 3-methylbutyl pentyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-266.82	kJ/mol	Joback Method
hf	-684.67	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.237		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	2225.00		NIST Webbook
tb	795.04	K	Joback Method
tc	997.07	K	Joback Method
tf	460.88	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.78	J/molxK	795.04	Joback Method
cpg	830.46	J/molxK	963.40	Joback Method
cpg	818.82	J/molxK	929.73	Joback Method
cpg	806.14	J/molxK	896.06	Joback Method
cpg	792.42	J/molxK	862.38	Joback Method
cpg	777.64	J/molxK	828.71	Joback Method
cpg	841.10	J/molxK	997.07	Joback Method
dvisc	0.0000662	Paxs	795.04	Joback Method
dvisc	0.0000860	Paxs	739.35	Joback Method

dvisc	0.0001165	Paxs	683.65	Joback Method
dvisc	0.0001668	Paxs	627.96	Joback Method
dvisc	0.0002558	Paxs	572.27	Joback Method
dvisc	0.0004305	Paxs	516.57	Joback Method
dvisc	0.0008214	Paxs	460.88	Joback Method

Sources

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=U356459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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