

Terephthalic acid, isobutyl 3-methylbutyl ester

Inchi:	InChI=1S/C17H24O4/c1-12(2)9-10-20-16(18)14-5-7-15(8-6-14)17(19)21-11-13(3)4/h5-8,
InchiKey:	OCKWJROMQCZKLM-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CC(C)CCOC(=O)c1ccc(C(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-277.68	kJ/mol	Joback Method
hf	-669.31	kJ/mol	Joback Method
hfus	31.97	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.702		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
rinsol	2086.00		NIST Webbook
tb	771.72	K	Joback Method
tc	977.62	K	Joback Method
tf	434.61	K	Joback Method
vc	0.915	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.43	J/molxK	771.72	Joback Method
cpg	721.28	J/molxK	806.04	Joback Method
cpg	736.04	J/molxK	840.35	Joback Method
cpg	749.74	J/molxK	874.67	Joback Method
cpg	762.38	J/molxK	908.99	Joback Method
cpg	773.98	J/molxK	943.31	Joback Method
cpg	784.57	J/molxK	977.62	Joback Method
dvisc	0.0010554	Paxs	434.61	Joback Method
dvisc	0.0005175	Paxs	490.80	Joback Method

dvisc	0.0002938	Paxs	546.98	Joback Method
dvisc	0.0001853	Paxs	603.16	Joback Method
dvisc	0.0001265	Paxs	659.35	Joback Method
dvisc	0.0000916	Paxs	715.54	Joback Method
dvisc	0.0000696	Paxs	771.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356134&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

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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