

Terephthalic acid, 4,4-dimethylpent-2-yl isobutyl ester

Inchi:	InChI=1S/C19H28O4/c1-7-16(19(4,5)6)23-18(21)15-10-8-14(9-11-15)17(20)22-12-13(2)3
InchiKey:	TXWWGIVPOCTAEF-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCC(OC(=O)c1ccc(C(=O)OCC(C)C)cc1)C(C)(C)C
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-258.00	kJ/mol	Joback Method
hf	-719.34	kJ/mol	Joback Method
hfus	29.73	kJ/mol	Joback Method
hvap	77.07	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.481		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinsol	2192.00		NIST Webbook
tb	814.25	K	Joback Method
tc	1024.95	K	Joback Method
tf	459.57	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.42	J/molxK	814.25	Joback Method
cpg	837.92	J/molxK	849.37	Joback Method
cpg	853.22	J/molxK	884.48	Joback Method
cpg	867.36	J/molxK	919.60	Joback Method
cpg	880.38	J/molxK	954.72	Joback Method
cpg	892.31	J/molxK	989.84	Joback Method
cpg	903.21	J/molxK	1024.95	Joback Method
dvisc	0.0008259	Paxs	459.57	Joback Method
dvisc	0.0003796	Paxs	518.68	Joback Method

dvisc	0.0002046	Paxs	577.80	Joback Method
dvisc	0.0001236	Paxs	636.91	Joback Method
dvisc	0.0000814	Paxs	696.02	Joback Method
dvisc	0.0000572	Paxs	755.14	Joback Method
dvisc	0.0000423	Paxs	814.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415966&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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