

Terephthalic acid, di(2-methylpent-3-yl) ester

Inchi:	InChI=1S/C20H30O4/c1-7-17(13(3)4)23-19(21)15-9-11-16(12-10-15)20(22)24-18(8-2)14
InchiKey:	NJBDOINDJMEHLD-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCC(OC(=O)c1ccc(C(=O)OC(CC)C(C)C)cc1)C(C)C
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-257.30	kJ/mol	Joback Method
hf	-741.79	kJ/mol	Joback Method
hfus	32.69	kJ/mol	Joback Method
hvap	79.81	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.869		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinsol	2209.00		NIST Webbook
tb	839.48	K	Joback Method
tc	1047.32	K	Joback Method
tf	438.42	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.79	J/molxK	839.48	Joback Method
cpg	896.49	J/molxK	874.12	Joback Method
cpg	911.94	J/molxK	908.76	Joback Method
cpg	926.15	J/molxK	943.40	Joback Method
cpg	939.15	J/molxK	978.04	Joback Method
cpg	950.96	J/molxK	1012.68	Joback Method
cpg	961.60	J/molxK	1047.32	Joback Method
dvisc	0.0010900	Paxs	438.42	Joback Method
dvisc	0.0004325	Paxs	505.26	Joback Method

dvisc	0.0002129	Paxs	572.11	Joback Method
dvisc	0.0001216	Paxs	638.95	Joback Method
dvisc	0.0000772	Paxs	705.79	Joback Method
dvisc	0.0000530	Paxs	772.64	Joback Method
dvisc	0.0000387	Paxs	839.48	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=U356192&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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