

Isophthalic acid, 3,3-dimethylbut-2-yl hexyl ester

Inchi:	InChI=1S/C20H30O4/c1-6-7-8-9-13-23-18(21)16-11-10-12-17(14-16)19(22)24-15(2)20(3)
InchiKey:	GYEUYTUDVHNSIQ-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)(C)C)c1
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-247.14	kJ/mol	Joback Method
hf	-734.70	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	79.68	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.015		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinsol	2289.00		NIST Webbook
tb	837.57	K	Joback Method
tc	1044.90	K	Joback Method
tf	485.84	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.27	J/molxK	837.57	Joback Method
cpg	895.72	J/molxK	872.13	Joback Method
cpg	910.98	J/molxK	906.68	Joback Method
cpg	925.11	J/molxK	941.24	Joback Method
cpg	938.13	J/molxK	975.79	Joback Method
cpg	950.10	J/molxK	1010.35	Joback Method
cpg	961.05	J/molxK	1044.90	Joback Method
dvisc	0.0006273	Paxs	485.84	Joback Method
dvisc	0.0003093	Paxs	544.46	Joback Method

dvisc	0.0001750	Paxs	603.08	Joback Method
dvisc	0.0001095	Paxs	661.70	Joback Method
dvisc	0.0000740	Paxs	720.33	Joback Method
dvisc	0.0000530	Paxs	778.95	Joback Method
dvisc	0.0000398	Paxs	837.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356551&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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