

Isophthalic acid, 3-phenylpropyl propyl ester

Inchi:	InChI=1S/C20H22O4/c1-2-13-23-19(21)17-11-6-12-18(15-17)20(22)24-14-7-10-16-8-4-3
InchiKey:	VOBKIGDBPMWSFZ-UHFFFAOYSA-N
Formula:	C20H22O4
SMILES:	CCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]:	326.39

Physical Properties

Property code	Value	Unit	Source
gf	-135.13	kJ/mol	Joback Method
hf	-484.14	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	83.64	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.043		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2692.00		NIST Webbook
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tb	867.92	K	Joback Method
tc	1091.70	K	Joback Method
tf	524.84	K	Joback Method
vc	0.988	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.49	J/molxK	867.92	Joback Method
cpg	795.69	J/molxK	905.22	Joback Method
cpg	808.60	J/molxK	942.51	Joback Method
cpg	820.28	J/molxK	979.81	Joback Method
cpg	830.75	J/molxK	1017.10	Joback Method
cpg	840.06	J/molxK	1054.40	Joback Method
cpg	848.25	J/molxK	1091.70	Joback Method
dvisc	0.0005161	Paxs	524.84	Joback Method

dvisc	0.0002974	Paxs	582.02	Joback Method
dvisc	0.0001891	Paxs	639.20	Joback Method
dvisc	0.0001295	Paxs	696.38	Joback Method
dvisc	0.0000939	Paxs	753.56	Joback Method
dvisc	0.0000713	Paxs	810.74	Joback Method
dvisc	0.0000561	Paxs	867.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344386&Units=SI

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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