

Isophthalic acid, 2-biphenyl heptyl ester

Inchi:	InChI=1S/C27H28O4/c1-2-3-4-5-11-19-30-26(28)22-15-12-16-23(20-22)27(29)31-25-18-
InchiKey:	LLCQZYUIVMHZKE-UHFFFAOYSA-N
Formula:	C27H28O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1
Mol. weight [g/mol]:	416.51

Physical Properties

Property code	Value	Unit	Source
gf	26.59	kJ/mol	Joback Method
hf	-403.56	kJ/mol	Joback Method
hfus	52.60	kJ/mol	Joback Method
hvap	102.16	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	6.700		Crippen Method
mcvol	334.890	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinsol	3322.00		NIST Webbook
tb	1059.74	K	Joback Method
tc	1304.65	K	Joback Method
tf	642.67	K	Joback Method
vc	1.272	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.84	J/molxK	1059.74	Joback Method
cpg	1097.63	J/molxK	1100.56	Joback Method
cpg	1107.91	J/molxK	1141.38	Joback Method
cpg	1116.76	J/molxK	1182.20	Joback Method
cpg	1124.27	J/molxK	1223.02	Joback Method
cpg	1130.51	J/molxK	1263.83	Joback Method
cpg	1135.59	J/molxK	1304.65	Joback Method
dvisc	0.0001956	Paxs	642.67	Joback Method
dvisc	0.0001134	Paxs	712.18	Joback Method

dvisc	0.0000725	Paxs	781.69	Joback Method
dvisc	0.0000498	Paxs	851.21	Joback Method
dvisc	0.0000362	Paxs	920.72	Joback Method
dvisc	0.0000276	Paxs	990.23	Joback Method
dvisc	0.0000217	Paxs	1059.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344562&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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