

Isophthalic acid, 2-biphenyl butyl ester

Inchi:	InChI=1S/C24H22O4/c1-2-3-16-27-23(25)19-12-9-13-20(17-19)24(26)28-22-15-8-7-14-2
InchiKey:	DVFPWSYXDZJVJV-UHFFFAOYSA-N
Formula:	C24H22O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1
Mol. weight [g/mol]:	374.43

Physical Properties

Property code	Value	Unit	Source
gf	1.33	kJ/mol	Joback Method
hf	-341.64	kJ/mol	Joback Method
hfus	44.83	kJ/mol	Joback Method
hvap	95.48	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	5.530		Crippen Method
mvol	292.620	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	3020.00		NIST Webbook
tb	991.10	K	Joback Method
tc	1236.66	K	Joback Method
tf	608.86	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.17	J/molxK	991.10	Joback Method
cpg	953.65	J/molxK	1195.74	Joback Method
cpg	947.25	J/molxK	1154.81	Joback Method
cpg	939.57	J/molxK	1113.88	Joback Method
cpg	930.55	J/molxK	1072.95	Joback Method
cpg	920.10	J/molxK	1032.03	Joback Method
cpg	958.84	J/molxK	1236.66	Joback Method
dvisc	0.0000338	Paxs	991.10	Joback Method
dvisc	0.0000424	Paxs	927.39	Joback Method

dvisc	0.0000552	Paxs	863.69	Joback Method
dvisc	0.0000749	Paxs	799.98	Joback Method
dvisc	0.0001070	Paxs	736.27	Joback Method
dvisc	0.0001637	Paxs	672.57	Joback Method
dvisc	0.0002738	Paxs	608.86	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=U344559&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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