Isophthalic acid, 2-biphenyl propyl ester

Inchi: InChI=1S/C23H20O4/c1-2-15-26-22(24)18-11-8-12-19(16-18)23(25)27-21-14-7-6-13-20(

InchiKey: ZWOMGXOTRHADGC-UHFFFAOYSA-N

Formula: C23H20O4

SMILES: CCCOC(=O)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1

Mol. weight [g/mol]: 360.40

Physical Properties

Property code	Value	Unit	Source
gf	-7.09	kJ/mol	Joback Method
hf	-321.00	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	93.26	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	5.140		Crippen Method
mcvol	278.530	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	2900.00		NIST Webbook
rinpol	2900.00		NIST Webbook
tb	968.22	K	Joback Method
tc	1215.77	K	Joback Method
tf	597.59	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.94	J/mol×K	968.22	Joback Method
cpg	861.92	J/mol×K	1009.48	Joback Method
cpg	872.40	J/mol×K	1050.74	Joback Method
cpg	881.46	J/mol×K	1091.99	Joback Method
cpg	889.16	J/mol×K	1133.25	Joback Method
cpg	895.58	J/mol×K	1174.51	Joback Method
cpg	900.77	J/mol×K	1215.77	Joback Method
dvisc	0.0003043	Pa×s	597.59	Joback Method

dvisc	0.0001840	Pa×s	659.36	Joback Method
dvisc	0.0001212	Pa×s	721.13	Joback Method
dvisc	0.0000853	Pa×s	782.90	Joback Method
dvisc	0.0000632	Pa×s	844.68	Joback Method
dvisc	0.0000488	Pa×s	906.45	Joback Method
dvisc	0.0000389	Pa×s	968.22	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=U344557&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