Adipic acid, 4-biphenyl isobutyl ester

Inchi: InChI=1S/C22H26O4/c1-17(2)16-25-21(23)10-6-7-11-22(24)26-20-14-12-19(13-15-20)18
InchiKey: JVJMQLBSUNZDIJ-UHFFFAOYSA-N
Formula: C22H26O4
SMILES: CC(C)COC(=O)CCCCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-120.73	kJ/mol	Joback Method
hf	-530.70	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	87.70	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.019		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2821.00		NIST Webbook
rinpol	2821.00		NIST Webbook
tb	913.24	K	Joback Method
tc	1137.15	K	Joback Method
tf	532.38	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.33	J/mol×K	913.24	Joback Method
cpg	957.39	J/mol×K	1099.83	Joback Method
cpg	948.11	J/mol×K	1062.51	Joback Method
cpg	937.62	J/mol×K	1025.20	Joback Method
cpg	925.85	J/mol×K	987.88	Joback Method
cpg	912.77	J/mol×K	950.56	Joback Method
cpg	965.49	J/mol×K	1137.15	Joback Method
dvisc	0.0000388	Pa×s	913.24	Joback Method

dvisc	0.0000502	Pa×s	849.76	Joback Method
dvisc	0.0000679	Pa×s	786.29	Joback Method
dvisc	0.0000968	Pa×s	722.81	Joback Method
dvisc	0.0001477	Pa×s	659.33	Joback Method
dvisc	0.0002465	Pa×s	595.86	Joback Method
dvisc	0.0004650	Pa×s	532.38	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=U353922&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