Adipic acid, 4-biphenyl octyl ester

Inchi: InChI=1S/C26H34O4/c1-2-3-4-5-6-12-21-29-25(27)15-10-11-16-26(28)30-24-19-17-23(1
InchiKey: OYLNDODAEFJHLP-UHFFFAOYSA-N
Formula: C26H34O4
SMILES: CCCCCCCCOC(=O)CCCCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
gf	-84.61	kJ/mol	Joback Method
hf	-607.98	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	97.00	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.723		Crippen Method
mcvol	344.560	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	3310.00		NIST Webbook
rinpol	3310.00		NIST Webbook
tb	1005.20	K	Joback Method
tc	1232.41	K	Joback Method
tf	592.46	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.76	J/mol×K	1005.20	Joback Method
cpg	1196.71	J/mol×K	1194.54	Joback Method
cpg	1187.59	J/mol×K	1156.67	Joback Method
cpg	1177.21	J/mol×K	1118.81	Joback Method
cpg	1165.48	J/mol×K	1080.94	Joback Method
cpg	1152.36	J/mol×K	1043.07	Joback Method
cpg	1204.61	J/mol×K	1232.41	Joback Method
dvisc	0.0000236	Pa×s	1005.20	Joback Method

dvisc	0.0000305	Pa×s	936.41	Joback Method
dvisc	0.0000411	Pa×s	867.62	Joback Method
dvisc	0.0000582	Pa×s	798.83	Joback Method
dvisc	0.0000881	Pa×s	730.04	Joback Method
dvisc	0.0001452	Pa×s	661.25	Joback Method
dvisc	0.0002690	Pa×s	592.46	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=U353928&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