

Adipic acid, 4-biphenyl isohexyl ester

Inchi:	InChI=1S/C24H30O4/c1-19(2)9-8-18-27-23(25)12-6-7-13-24(26)28-22-16-14-21(15-17-2
InchiKey:	SJYAWYNAJSLLDW-UHFFFAOYSA-N
Formula:	C24H30O4
SMILES:	CC(C)CCCOC(=O)CCCCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	382.49

Physical Properties

Property code	Value	Unit	Source
gf	-103.89	kJ/mol	Joback Method
hf	-571.98	kJ/mol	Joback Method
hfus	47.66	kJ/mol	Joback Method
hvap	92.16	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	5.799		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	3060.00		NIST Webbook
rinpol	3060.00		NIST Webbook
tb	959.00	K	Joback Method
tc	1183.19	K	Joback Method
tf	554.92	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.17	J/mol×K	959.00	Joback Method
cpg	1076.05	J/mol×K	1145.83	Joback Method
cpg	1066.89	J/mol×K	1108.46	Joback Method
cpg	1056.47	J/mol×K	1071.10	Joback Method
cpg	1044.74	J/mol×K	1033.73	Joback Method
cpg	1031.66	J/mol×K	996.37	Joback Method
cpg	1084.02	J/mol×K	1183.19	Joback Method
dvisc	0.0000290	Pa×s	959.00	Joback Method

dvisc	0.0000377	Pa×s	891.65	Joback Method
dvisc	0.0000514	Pa×s	824.31	Joback Method
dvisc	0.0000738	Pa×s	756.96	Joback Method
dvisc	0.0001139	Pa×s	689.61	Joback Method
dvisc	0.0001929	Pa×s	622.27	Joback Method
dvisc	0.0003715	Pa×s	554.92	Joback Method

Sources

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=U353925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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