

Dodecanoic acid, 4-biphenyl ester

Inchi: InChI=1S/C24H32O2/c1-2-3-4-5-6-7-8-9-13-16-24(25)26-23-19-17-22(18-20-23)21-14-11
InchiKey: LCRGZXAZWAIIGQ-UHFFFAOYSA-N
Formula: C24H32O2
SMILES: CCCCCCCCCCCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	132.47	kJ/mol	Joback Method
hf	-321.90	kJ/mol	Joback Method
hfus	48.40	kJ/mol	Joback Method
hvap	83.39	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	7.180		Crippen Method
mcvol	308.940	ml/mol	McGowan Method
pc	1249.49	kPa	Joback Method
rinpol	2935.00		NIST Webbook
tb	883.15	K	Joback Method
tc	1096.86	K	Joback Method
tf	497.76	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.97	J/mol×K	883.15	Joback Method
cpg	1047.26	J/mol×K	1061.24	Joback Method
cpg	1034.66	J/mol×K	1025.62	Joback Method
cpg	1020.99	J/mol×K	990.00	Joback Method
cpg	1006.20	J/mol×K	954.39	Joback Method
cpg	990.21	J/mol×K	918.77	Joback Method
cpg	1058.86	J/mol×K	1096.86	Joback Method
dvisc	0.0000446	Pa×s	883.15	Joback Method
dvisc	0.0000579	Pa×s	818.92	Joback Method

dvisc	0.0000787	Pa×s	754.69	Joback Method
dvisc	0.0001133	Pa×s	690.45	Joback Method
dvisc	0.0001757	Pa×s	626.22	Joback Method
dvisc	0.0003013	Pa×s	561.99	Joback Method
dvisc	0.0005938	Pa×s	497.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U360551&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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