

Succinic acid, 4-biphenyl octyl ester

Inchi:	InChI=1S/C24H30O4/c1-2-3-4-5-6-10-19-27-23(25)17-18-24(26)28-22-15-13-21(14-16-2
InchiKey:	NGMNEPDWPHKAMO-UHFFFAOYSA-N
Formula:	C24H30O4
SMILES:	CCCCCCCCOC(=O)CCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	382.49

Physical Properties

Property code	Value	Unit	Source
gf	-101.45	kJ/mol	Joback Method
hf	-566.70	kJ/mol	Joback Method
hfus	51.18	kJ/mol	Joback Method
hvap	92.54	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	5.943		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinsol	3068.00		NIST Webbook
tb	959.44	K	Joback Method
tc	1182.13	K	Joback Method
tf	569.92	K	Joback Method
vc	1.212	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.74	J/molxK	959.44	Joback Method
cpg	1031.19	J/molxK	996.55	Joback Method
cpg	1044.26	J/molxK	1033.67	Joback Method
cpg	1056.00	J/molxK	1070.78	Joback Method
cpg	1066.47	J/molxK	1107.90	Joback Method
cpg	1075.71	J/molxK	1145.01	Joback Method
cpg	1083.79	J/molxK	1182.13	Joback Method
dvisc	0.0003390	Paxs	569.92	Joback Method
dvisc	0.0001867	Paxs	634.84	Joback Method

dvisc	0.0001149	Paxs	699.76	Joback Method
dvisc	0.0000768	Paxs	764.68	Joback Method
dvisc	0.0000547	Paxs	829.60	Joback Method
dvisc	0.0000409	Paxs	894.52	Joback Method
dvisc	0.0000318	Paxs	959.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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