

Sebacic acid, diphenyl ester

Inchi:	InChI=1S/C22H26O4/c23-21(25-19-13-7-5-8-14-19)17-11-3-1-2-4-12-18-22(24)26-20-15
InchiKey:	ODVYFOLTLWONHF-UHFFFAOYSA-N
Formula:	C22H26O4
SMILES:	O=C(CCCCCCCC(=O)Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	354.44

Physical Properties

Property code	Value	Unit	Source
gf	-108.66	kJ/mol	Joback Method
hf	-513.95	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	87.43	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.318		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1506.98	kPa	Joback Method
rinsol	2936.00		NIST Webbook
tb	908.70	K	Joback Method
tc	1129.57	K	Joback Method
tf	534.86	K	Joback Method
vc	1.099	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.88	J/molxK	908.70	Joback Method
cpg	958.54	J/molxK	1092.76	Joback Method
cpg	949.02	J/molxK	1055.95	Joback Method
cpg	938.34	J/molxK	1019.14	Joback Method
cpg	926.46	J/molxK	982.32	Joback Method
cpg	913.32	J/molxK	945.51	Joback Method
cpg	966.97	J/molxK	1129.57	Joback Method
dvisc	0.0000417	Paxs	908.70	Joback Method
dvisc	0.0000539	Paxs	846.39	Joback Method

dvisc	0.0000727	Paxs	784.09	Joback Method
dvisc	0.0001033	Paxs	721.78	Joback Method
dvisc	0.0001567	Paxs	659.47	Joback Method
dvisc	0.0002594	Paxs	597.17	Joback Method
dvisc	0.0004828	Paxs	534.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354521&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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