

Butanedioic acid, 2,3-diphenyl-

Other names:	2,3-Diphenylsuccinic acid Succinic acid, 2,3-diphenyl- «alpha», «beta»-Diphenylsuccinic acid Racemic-2,3-diphenylbutanedioic acid
Inchi:	InChI=1S/C16H14O4/c17-15(18)13(11-7-3-1-4-8-11)14(16(19)20)12-9-5-2-6-10-12/h1-10
InchiKey:	PVXCQHHWNDJIJP-UHFFFAOYSA-N
Formula:	C16H14O4
SMILES:	O=C(O)C(c1ccccc1)C(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	270.28
CAS:	7584-72-7

Physical Properties

Property code	Value	Unit	Source
chs	-7556.80 ± 3.80	kJ/mol	NIST Webbook
gf	-227.70	kJ/mol	Joback Method
hf	-440.69	kJ/mol	Joback Method
hfus	29.61	kJ/mol	Joback Method
hvap	101.84	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.723		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
tb	910.06	K	Joback Method
tc	1132.47	K	Joback Method
tf	514.42	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.65	J/molxK	910.06	Joback Method
cpg	641.64	J/molxK	1095.40	Joback Method
cpg	635.32	J/molxK	1058.34	Joback Method
cpg	628.43	J/molxK	1021.27	Joback Method

cpg	620.90	J/molxK	984.20	Joback Method
cpg	612.66	J/molxK	947.13	Joback Method
cpg	647.47	J/molxK	1132.47	Joback Method
dvisc	0.0000029	Paxs	910.06	Joback Method
dvisc	0.0000047	Paxs	844.12	Joback Method
dvisc	0.0000086	Paxs	778.18	Joback Method
dvisc	0.0000173	Paxs	712.24	Joback Method
dvisc	0.0000401	Paxs	646.30	Joback Method
dvisc	0.0001130	Paxs	580.36	Joback Method
dvisc	0.0004152	Paxs	514.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7584727&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

chs:	Standard solid enthalpy of combustion
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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