

Butanedioic acid, phenyl-

Other names:	Succinic acid, phenyl- «alpha»-Phenylsuccinic acid Phenylsuccinic acid 2-Phenylsuccinic acid dl-Phenylsuccinic acid
Inchi:	InChI=1S/C10H10O4/c11-9(12)6-8(10(13)14)7-4-2-1-3-5-7/h1-5,8H,6H2,(H,11,12)(H,13,
InchiKey:	LVFFZQQWIZURIO-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	O=C(O)CC(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	194.18
CAS:	635-51-8

Physical Properties

Property code	Value	Unit	Source
chs	-4523.30 ± 2.30	kJ/mol	NIST Webbook
gf	-388.19	kJ/mol	Joback Method
hf	-548.10	kJ/mol	Joback Method
hfus	23.55	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.329		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
tb	746.54	K	Joback Method
tc	946.57	K	Joback Method
tf	435.38	K	Joback Method
vc	0.531	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.78	J/mol×K	746.54	Joback Method
cpg	391.95	J/mol×K	779.88	Joback Method
cpg	399.54	J/mol×K	813.22	Joback Method

cpg	406.58	J/mol×K	846.55	Joback Method
cpg	413.09	J/mol×K	879.89	Joback Method
cpg	419.10	J/mol×K	913.23	Joback Method
cpg	424.64	J/mol×K	946.57	Joback Method
dvisc	0.0018592	Paxs	435.38	Joback Method
dvisc	0.0005145	Paxs	487.24	Joback Method
dvisc	0.0001823	Paxs	539.10	Joback Method
dvisc	0.0000775	Paxs	590.96	Joback Method
dvisc	0.0000378	Paxs	642.82	Joback Method
dvisc	0.0000205	Paxs	694.68	Joback Method
dvisc	0.0000121	Paxs	746.54	Joback Method
hfust	37.37	kJ/mol	440.10	NIST Webbook

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=C635518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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