

«alpha»-Benzylsuccinic acid

Other names:	Benzenebutanoic acid, «beta»-carboxy-
Inchi:	InChI=1S/C11H12O4/c12-10(13)7-9(11(14)15)6-8-4-2-1-3-5-8/h1-5,9H,6-7H2,(H,12,13)(H,14,15)
InchiKey:	GTOFKXZQQDSVFH-UHFFFAOYSA-N
Formula:	C11H12O4
SMILES:	O=C(O)CC(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	208.21
CAS:	884-33-3

Physical Properties

Property code	Value	Unit	Source
gf	-379.77	kJ/mol	Joback Method
hf	-568.74	kJ/mol	Joback Method
hfus	26.14	kJ/mol	Joback Method
hvap	88.82	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.405		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	769.42	K	Joback Method
tc	968.23	K	Joback Method
tf	446.65	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.85	J/mol×K	769.42	Joback Method
cpg	443.62	J/mol×K	802.56	Joback Method
cpg	451.78	J/mol×K	835.69	Joback Method
cpg	459.35	J/mol×K	868.83	Joback Method
cpg	466.37	J/mol×K	901.96	Joback Method
cpg	472.87	J/mol×K	935.10	Joback Method
cpg	478.89	J/mol×K	968.23	Joback Method
dvisc	0.0014876	Pa×s	446.65	Joback Method

dvisc	0.0004106	Pa×s	500.44	Joback Method
dvisc	0.0001455	Pa×s	554.24	Joback Method
dvisc	0.0000619	Pa×s	608.03	Joback Method
dvisc	0.0000303	Pa×s	661.83	Joback Method
dvisc	0.0000165	Pa×s	715.62	Joback Method
dvisc	0.0000098	Pa×s	769.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C884333&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/68-663-1/alpha-Benzylsuccinic-acid.pdf>

Generated by Cheméo on 2025-12-24 09:02:11.876084572 +0000 UTC m=+6315129.406125226.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.