

Benzeneacetic acid, «alpha»-methyl-, (S)-

Inchi:	InChI=1S/C9H10O2/c1-7(9(10)11)8-5-3-2-4-6-8/h2-7H,1H3,(H,10,11)/t7-m/s1
InchiKey:	YPGCWEMNNLXISK-SSDOTTSWSA-N
Formula:	C9H10O2
SMILES:	CC(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	150.17
CAS:	7782-24-3

Physical Properties

Property code	Value	Unit	Source
gf	-130.87	kJ/mol	Joback Method
hf	-262.65	kJ/mol	Joback Method
hfus	15.27	kJ/mol	Joback Method
hvap	60.94	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.875		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	577.61	K	Joback Method
tc	785.00	K	Joback Method
tf	313.36	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.79	J/molxK	577.61	Joback Method
cpg	329.12	J/molxK	750.43	Joback Method
cpg	320.91	J/molxK	715.87	Joback Method
cpg	312.10	J/molxK	681.30	Joback Method
cpg	302.67	J/molxK	646.74	Joback Method
cpg	292.57	J/molxK	612.17	Joback Method
cpg	336.75	J/molxK	785.00	Joback Method
dvisc	0.0001014	Paxs	577.61	Joback Method
dvisc	0.0001602	Paxs	533.57	Joback Method

dvisc	0.0002745	Paxs	489.53	Joback Method
dvisc	0.0005232	Paxs	445.49	Joback Method
dvisc	0.0011492	Paxs	401.44	Joback Method
dvisc	0.0030643	Paxs	357.40	Joback Method
dvisc	0.0107638	Paxs	313.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.20	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7782243&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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