

«beta», «beta»-dimethylbenzenepropionic acid

Inchi:	InChI=1S/C11H14O2/c1-11(2,10(12)13)8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3,(H,12,13)
InchiKey:	BQHWATVEWGHHHF-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CC(C)(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	178.23

Physical Properties

Property code	Value	Unit	Source
gf	-108.75	kJ/mol	Joback Method
hf	-307.40	kJ/mol	Joback Method
hfus	16.56	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.340		Crippen Method
mvol	149.530	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
ripol	2262.00		NIST Webbook
ripol	2262.00		NIST Webbook
tb	620.58	K	Joback Method
tc	829.07	K	Joback Method
tf	353.32	K	Joback Method
vc	0.557	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.97	J/mol×K	620.58	Joback Method
cpg	391.51	J/mol×K	655.33	Joback Method
cpg	403.17	J/mol×K	690.08	Joback Method
cpg	414.02	J/mol×K	724.82	Joback Method
cpg	424.10	J/mol×K	759.57	Joback Method
cpg	433.48	J/mol×K	794.32	Joback Method
cpg	442.20	J/mol×K	829.07	Joback Method
dvisc	0.0054910	Paxs	353.32	Joback Method

dvisc	0.0017627	Paxs	397.86	Joback Method
dvisc	0.0007113	Paxs	442.41	Joback Method
dvisc	0.0003389	Paxs	486.95	Joback Method
dvisc	0.0001828	Paxs	531.49	Joback Method
dvisc	0.0001085	Paxs	576.04	Joback Method
dvisc	0.0000694	Paxs	620.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R299013&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

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

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