Butanedioic acid, methyl phenylmethyl ester

Other names: Methyl benzyl succinate
Inchi: InChI=1S/C12H14O4/c1-15-11(13)7-8-12(14)16-9-10-5-3-2-4-6-10/h2-6H,7-9H2,1H3
InchiKey: MUXGHJRHNFYSBX-UHFFFAOYSA-N
Formula: C12H14O4
SMILES: COC(=O)CCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 222.24
CAS: 119450-11-2

Physical Properties

Property code	Value	Unit	Source
gf	-305.27	kJ/mol	Joback Method
hf	-544.08	kJ/mol	Joback Method
hfus	26.45	kJ/mol	Joback Method
hvap	62.89	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.683		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1636.00		NIST Webbook
tb	653.22	K	Joback Method
tc	864.17	K	Joback Method
tf	395.74	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.45	J/mol×K	653.22	Joback Method
cpg	450.97	J/mol×K	688.38	Joback Method
cpg	463.65	J/mol×K	723.54	Joback Method
cpg	475.50	J/mol×K	758.69	Joback Method
cpg	486.52	J/mol×K	793.85	Joback Method
cpg	496.72	J/mol×K	829.01	Joback Method
cpg	506.11	J/mol×K	864.17	Joback Method

dvisc	0.0013619	Pa×s	395.74	Joback Method
dvisc	0.0007885	Pa×s	438.65	Joback Method
dvisc	0.0005033	Pa×s	481.57	Joback Method
dvisc	0.0003457	Pa×s	524.48	Joback Method
dvisc	0.0002514	Pa×s	567.39	Joback Method
dvisc	0.0001911	Pa×s	610.31	Joback Method
dvisc	0.0001507	Pa×s	653.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119450112&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume