

Succinic acid, bromo-, dimethyl ester

Inchi:	InChI=1S/C6H9BrO4/c1-10-5(8)3-4(7)6(9)11-2/h4H,3H2,1-2H3
InchiKey:	RGYMYJITHXYRMA-UHFFFAOYSA-N
Formula:	C6H9BrO4
SMILES:	COC(=O)CC(Br)C(=O)OC
Mol. weight [g/mol]:	225.04
CAS:	760-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-456.32	kJ/mol	Joback Method
hf	-635.72	kJ/mol	Joback Method
hfus	18.63	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-0.60		Crippen Method
logp	0.486		Crippen Method
mcvol	127.780	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	554.98	K	Joback Method
tc	761.15	K	Joback Method
tf	346.50	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.30	J/molxK	554.98	Joback Method
cpg	278.49	J/molxK	589.34	Joback Method
cpg	287.26	J/molxK	623.70	Joback Method
cpg	295.61	J/molxK	658.07	Joback Method
cpg	303.51	J/molxK	692.43	Joback Method
cpg	310.98	J/molxK	726.79	Joback Method
cpg	317.99	J/molxK	761.15	Joback Method
dvisc	0.0021068	Paxs	346.50	Joback Method
dvisc	0.0012666	Paxs	381.25	Joback Method

dvisc	0.0008290	Paxs	415.99	Joback Method
dvisc	0.0005793	Paxs	450.74	Joback Method
dvisc	0.0004261	Paxs	485.49	Joback Method
dvisc	0.0003265	Paxs	520.23	Joback Method
dvisc	0.0002587	Paxs	554.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C760907&Units=SI

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

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