Succinic acid, 2-bromophenethyl propyl ester

Inchi: InChI=1S/C15H19BrO4/c1-2-10-19-14(17)7-8-15(18)20-11-9-12-5-3-4-6-13(12)16/h3-6H
InchiKey: VDQNRXKQYSOOQP-UHFFFAOYSA-N
Formula: C15H19BrO4
SMILES: CCCOC(=O)CCC(=O)OCCc1ccccc1Br
Mol. weight [g/mol]: 343.21

Physical Properties

Property code	Value	Unit	Source
gf	-275.32	kJ/mol	Joback Method
hf	-591.14	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	76.67	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.268		Crippen Method
mcvol	230.830	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	2224.00		NIST Webbook
tb	793.00	K	Joback Method
tc	1006.77	K	Joback Method
tf	501.87	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.16	J/mol×K	793.00	Joback Method
cpg	688.74	J/mol×K	971.14	Joback Method
cpg	679.29	J/mol×K	935.51	Joback Method
cpg	668.93	J/mol×K	899.88	Joback Method
cpg	657.63	J/mol×K	864.26	Joback Method
cpg	645.38	J/mol×K	828.63	Joback Method
cpg	697.29	J/mol×K	1006.77	Joback Method
dvisc	0.0000885	Pa×s	793.00	Joback Method
dvisc	0.0001107	Pa×s	744.48	Joback Method

dvisc	0.0001429	Pa×s	695.96	Joback Method
dvisc	0.0001917	Pa×s	647.43	Joback Method
dvisc	0.0002696	Pa×s	598.91	Joback Method
dvisc	0.0004028	Pa×s	550.39	Joback Method
dvisc	0.0006502	Pa×s	501.87	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U381447&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume