Succinic acid, 2-bromophenethyl ethyl ester

Inchi: InChI=1S/C14H17BrO4/c1-2-18-13(16)7-8-14(17)19-10-9-11-5-3-4-6-12(11)15/h3-6H,2,7
InchiKey: YMWIJYGGRDRGDN-UHFFFAOYSA-N
Formula: C14H17BrO4
SMILES: CCOC(=O)CCC(=O)OCCc1ccccc1Br
Mol. weight [g/mol]: 329.19

Physical Properties

Property code	Value	Unit	Source
gf	-283.74	kJ/mol	Joback Method
hf	-570.50	kJ/mol	Joback Method
hfus	36.53	kJ/mol	Joback Method
hvap	74.44	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.878		Crippen Method
mcvol	216.740	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
tb	770.12	K	Joback Method
tc	986.25	K	Joback Method
tf	490.60	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.72	J/mol×K	770.12	Joback Method
cpg	590.59	J/mol×K	806.14	Joback Method
cpg	602.53	J/mol×K	842.16	Joback Method
cpg	613.53	J/mol×K	878.18	Joback Method
cpg	623.64	J/mol×K	914.21	Joback Method
cpg	632.85	J/mol×K	950.23	Joback Method
cpg	641.19	J/mol×K	986.25	Joback Method
dvisc	0.0007115	Pa×s	490.60	Joback Method

dvisc	0.0004468	Pa×s	537.19	Joback Method
dvisc	0.0003022	Pa×s	583.77	Joback Method
dvisc	0.0002166	Pa×s	630.36	Joback Method
dvisc	0.0001625	Pa×s	676.95	Joback Method
dvisc	0.0001265	Pa×s	723.53	Joback Method
dvisc	0.0001015	Pa×s	770.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381446&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