Succinic acid, 4-bromobenzyl ethyl ester

Inchi: InChI=1S/C13H15BrO4/c1-2-17-12(15)7-8-13(16)18-9-10-3-5-11(14)6-4-10/h3-6H,2,7-9H
InchiKey: ZNCLNYXXKDBRAW-UHFFFAOYSA-N
Formula: C13H15BrO4
SMILES: CCOC(=O)CCC(=O)OCc1ccc(Br)cc1
Mol. weight [g/mol]: 315.16

Physical Properties

Property code	Value	Unit	Source
gf	-292.16	kJ/mol	Joback Method
hf	-549.86	kJ/mol	Joback Method
hfus	33.94	kJ/mol	Joback Method
hvap	72.22	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.836		Crippen Method
mcvol	202.650	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	747.24	K	Joback Method
tc	966.26	K	Joback Method
tf	479.33	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.38	J/mol×K	747.24	Joback Method
cpg	536.84	J/mol×K	783.74	Joback Method
cpg	548.40	J/mol×K	820.25	Joback Method
cpg	559.06	J/mol×K	856.75	Joback Method
cpg	568.84	J/mol×K	893.25	Joback Method
cpg	577.76	J/mol×K	929.75	Joback Method
cpg	585.84	J/mol×K	966.26	Joback Method
dvisc	0.0007747	Pa×s	479.33	Joback Method

dvisc	0.0004934	Pa×s	523.98	Joback Method
dvisc	0.0003373	Pa×s	568.63	Joback Method
dvisc	0.0002437	Pa×s	613.29	Joback Method
dvisc	0.0001840	Pa×s	657.94	Joback Method
dvisc	0.0001440	Pa×s	702.59	Joback Method
dvisc	0.0001161	Pa×s	747.24	Joback Method

Sources

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=U382426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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