Succinic acid, 4-bromobenzyl pentyl ester

Inchi: InChI=1S/C16H21BrO4/c1-2-3-4-11-20-15(18)9-10-16(19)21-12-13-5-7-14(17)8-6-13/h5-
InchiKey: XNAVGPSLUOIRFF-UHFFFAOYSA-N
Formula: C16H21BrO4
SMILES: CCCCCOC(=O)CCC(=O)OCc1ccc(Br)cc1
Mol. weight [g/mol]: 357.24

Physical Properties

Property code	Value	Unit	Source
gf	-266.90	kJ/mol	Joback Method
hf	-611.78	kJ/mol	Joback Method
hfus	41.71	kJ/mol	Joback Method
hvap	78.90	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.006		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	815.88	K	Joback Method
tc	1027.86	K	Joback Method
tf	513.14	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.61	J/mol×K	815.88	Joback Method
cpg	701.14	J/mol×K	851.21	Joback Method
cpg	713.65	J/mol×K	886.54	Joback Method
cpg	725.19	J/mol×K	921.87	Joback Method
cpg	735.77	J/mol×K	957.20	Joback Method
cpg	745.41	J/mol×K	992.53	Joback Method
cpg	754.13	J/mol×K	1027.86	Joback Method
dvisc	0.0005914	Pa×s	513.14	Joback Method

dvisc	0.0003615	Pa×s	563.60	Joback Method
dvisc	0.0002396	Pa×s	614.05	Joback Method
dvisc	0.0001691	Pa×s	664.51	Joback Method
dvisc	0.0001253	Pa×s	714.97	Joback Method
dvisc	0.0000966	Pa×s	765.42	Joback Method
dvisc	0.0000769	Pa×s	815.88	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=U382429&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