Succinic acid, di(3-bromobenzyl) ester

Inchi: InChI=1S/C18H16Br2O4/c19-15-5-1-3-13(9-15)11-23-17(21)7-8-18(22)24-12-14-4-2-6-16(20)10-14/h1-6,9-10H,7-8,11-12H2

InchiKey: MMXNQNZILSAQQK-UHFFFAOYSA-N

Formula: C18H16Br2O4

SMILES: O=C(CCC(=O)OCc1cccc(Br)c1)OCc1cccc(Br)c1

Mol. weight [g/mol]: 456.12

Physical Properties

Property code	Value	Unit	Source
gf	-132.96	kJ/mol	Joback Method
hf	-401.67	kJ/mol	Joback Method
hfus	45.82	kJ/mol	Joback Method
hvap	92.72	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	4.778		Crippen Method
mcvol	266.840	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	3005.00		NIST Webbook
rinpol	3005.00		NIST Webbook
tb	959.46	K	Joback Method
tc	1206.97	K	Joback Method
tf	634.42	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.10	J/mol×K	959.46	Joback Method
cpg	767.80	J/mol×K	1165.72	Joback Method
cpg	761.88	J/mol×K	1124.47	Joback Method
cpg	755.01	J/mol×K	1083.22	Joback Method
cpg	747.13	J/mol×K	1041.96	Joback Method
cpg	738.18	J/mol×K	1000.71	Joback Method
cpg	772.83	J/mol×K	1206.97	Joback Method
dvisc	0.0000465	Pa×s	959.46	Joback Method

dvisc	0.0000570	Pa×s	905.29	Joback Method
dvisc	0.0000717	Pa×s	851.11	Joback Method
dvisc	0.0000932	Pa×s	796.94	Joback Method
dvisc	0.0001258	Pa×s	742.77	Joback Method
dvisc	0.0001779	Pa×s	688.59	Joback Method
dvisc	0.0002671	Pa×s	634.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382425&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

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

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