

Succinic acid, di(2-bromobenzyl) ester

Inchi: InChI=1S/C18H16Br2O4/c19-15-7-3-1-5-13(15)11-23-17(21)9-10-18(22)24-12-14-6-2-4-
InchiKey: AQWCKCLHDBQTGB-UHFFFAOYSA-N
Formula: C18H16Br2O4
SMILES: O=C(CCC(=O)OCc1ccccc1Br)OCc1ccccc1Br
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
mvol	266.840	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	2950.00		NIST Webbook
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tb	959.46	K	Joback Method
tc	1206.97	K	Joback Method
tf	634.42	K	Joback Method
vc	1.000	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.10	J/molxK	959.46	Joback Method
cpg	738.18	J/molxK	1000.71	Joback Method
cpg	747.13	J/molxK	1041.96	Joback Method
cpg	755.01	J/molxK	1083.22	Joback Method
cpg	761.88	J/molxK	1124.47	Joback Method
cpg	767.80	J/molxK	1165.72	Joback Method
cpg	772.83	J/molxK	1206.97	Joback Method
dvisc	0.0002671	Paxs	634.42	Joback Method

dvisc	0.0001779	Paxs	688.59	Joback Method
dvisc	0.0001258	Paxs	742.77	Joback Method
dvisc	0.0000932	Paxs	796.94	Joback Method
dvisc	0.0000717	Paxs	851.11	Joback Method
dvisc	0.0000570	Paxs	905.29	Joback Method
dvisc	0.0000465	Paxs	959.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U381125&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

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