

Succinic acid, 1-(3-bromophenyl)ethyl octyl ester

Inchi:	InChI=1S/C20H29BrO4/c1-3-4-5-6-7-8-14-24-19(22)12-13-20(23)25-16(2)17-10-9-11-18
InchiKey:	FDLKTQSLNZSHMG-UHFFFAOYSA-N
Formula:	C20H29BrO4
SMILES:	CCCCCCCCOC(=O)CCC(=O)OC(C)c1cccc(Br)c1
Mol. weight [g/mol]:	413.35

Physical Properties

Property code	Value	Unit	Source
gf	-235.66	kJ/mol	Joback Method
hf	-699.62	kJ/mol	Joback Method
hfus	48.54	kJ/mol	Joback Method
hvap	87.41	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.737		Crippen Method
mcvol	301.280	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2626.00		NIST Webbook
rinpol	2626.00		NIST Webbook
tb	906.96	K	Joback Method
tc	1119.93	K	Joback Method
tf	543.22	K	Joback Method
vc	1.151	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.65	J/molxK	906.96	Joback Method
cpg	933.17	J/molxK	942.46	Joback Method
cpg	946.52	J/molxK	977.95	Joback Method
cpg	958.72	J/molxK	1013.45	Joback Method
cpg	969.82	J/molxK	1048.94	Joback Method
cpg	979.85	J/molxK	1084.44	Joback Method
cpg	988.85	J/molxK	1119.93	Joback Method
dvisc	0.0004271	Paxs	543.22	Joback Method

dvisc	0.0002349	Paxs	603.84	Joback Method
dvisc	0.0001441	Paxs	664.47	Joback Method
dvisc	0.0000959	Paxs	725.09	Joback Method
dvisc	0.0000680	Paxs	785.71	Joback Method
dvisc	0.0000506	Paxs	846.34	Joback Method
dvisc	0.0000392	Paxs	906.96	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=U381469&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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