

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

Inchi:	InChI=1S/C18H25BrO4/c1-3-4-5-6-12-22-17(20)10-11-18(21)23-14(2)15-8-7-9-16(19)13
InchiKey:	FWYGWVQJCZZGHF-UHFFFAOYSA-N
Formula:	C18H25BrO4
SMILES:	CCCCCOC(=O)CCC(=O)OC(C)c1cccc(Br)c1
Mol. weight [g/mol]:	385.29

Physical Properties

Property code	Value	Unit	Source
gf	-252.50	kJ/mol	Joback Method
hf	-658.34	kJ/mol	Joback Method
hfus	43.36	kJ/mol	Joback Method
hvap	82.96	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.957		Crippen Method
mvol	273.100	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	2421.00		NIST Webbook
rinpol	2421.00		NIST Webbook
tb	861.20	K	Joback Method
tc	1073.69	K	Joback Method
tf	520.68	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.82	J/molxK	861.20	Joback Method
cpg	815.96	J/molxK	896.62	Joback Method
cpg	829.00	J/molxK	932.03	Joback Method
cpg	840.97	J/molxK	967.45	Joback Method
cpg	851.89	J/molxK	1002.86	Joback Method
cpg	861.79	J/molxK	1038.28	Joback Method
cpg	870.71	J/molxK	1073.69	Joback Method
dvisc	0.0005342	Paxs	520.68	Joback Method

dvisc	0.0003006	Paxs	577.43	Joback Method
dvisc	0.0001875	Paxs	634.19	Joback Method
dvisc	0.0001263	Paxs	690.94	Joback Method
dvisc	0.0000904	Paxs	747.69	Joback Method
dvisc	0.0000678	Paxs	804.45	Joback Method
dvisc	0.0000528	Paxs	861.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381467&Units=SI
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

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
mccvol:	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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