

Succinic acid, 4-bromobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H25BrO4/c1-4-5-16(13(2)3)23-18(21)11-10-17(20)22-12-14-6-8-15(19)9-7
InchiKey:	ZPMALPDWHDZQEF-UHFFFAOYSA-N
Formula:	C18H25BrO4
SMILES:	CCCC(OC(=O)CCC(=O)OCc1ccc(Br)cc1)C(C)C
Mol. weight [g/mol]:	385.29

Physical Properties

Property code	Value	Unit	Source
gf	-254.94	kJ/mol	Joback Method
hf	-663.62	kJ/mol	Joback Method
hfus	39.84	kJ/mol	Joback Method
hvap	82.57	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.640		Crippen Method
mvol	273.100	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook
tb	860.76	K	Joback Method
tc	1075.59	K	Joback Method
tf	505.68	K	Joback Method
vc	1.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.36	J/molxK	860.76	Joback Method
cpg	816.64	J/molxK	896.56	Joback Method
cpg	829.78	J/molxK	932.37	Joback Method
cpg	841.80	J/molxK	968.17	Joback Method
cpg	852.75	J/molxK	1003.98	Joback Method
cpg	862.65	J/molxK	1039.78	Joback Method
cpg	871.52	J/molxK	1075.59	Joback Method
dvisc	0.0005989	Paxs	505.68	Joback Method

dvisc	0.0003161	Paxs	564.86	Joback Method
dvisc	0.0001883	Paxs	624.04	Joback Method
dvisc	0.0001227	Paxs	683.22	Joback Method
dvisc	0.0000856	Paxs	742.40	Joback Method
dvisc	0.0000630	Paxs	801.58	Joback Method
dvisc	0.0000484	Paxs	860.76	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=U382430&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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