

Succinic acid, 2-methoxybenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C19H28O5/c1-5-8-16(14(2)3)24-19(21)12-11-18(20)23-13-15-9-6-7-10-17(15)2
InchiKey:	BHTISPPVPNSKPB-UHFFFAOYSA-N
Formula:	C19H28O5
SMILES:	CCCC(OC(=O)CCC(=O)OCc1ccccc1OC)C(C)C
Mol. weight [g/mol]:	336.42

Physical Properties

Property code	Value	Unit	Source
gf	-365.84	kJ/mol	Joback Method
hf	-842.81	kJ/mol	Joback Method
hfus	38.33	kJ/mol	Joback Method
hvap	80.77	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.886		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2326.00		NIST Webbook
tb	839.90	K	Joback Method
tc	1044.02	K	Joback Method
tf	479.38	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.22	J/molxK	839.90	Joback Method
cpg	915.68	J/molxK	1010.00	Joback Method
cpg	904.79	J/molxK	975.98	Joback Method
cpg	892.71	J/molxK	941.96	Joback Method
cpg	879.43	J/molxK	907.94	Joback Method
cpg	864.93	J/molxK	873.92	Joback Method
cpg	925.38	J/molxK	1044.02	Joback Method
dvisc	0.0000398	Paxs	839.90	Joback Method
dvisc	0.0000525	Paxs	779.81	Joback Method

dvisc	0.0000725	Paxs	719.73	Joback Method
dvisc	0.0001062	Paxs	659.64	Joback Method
dvisc	0.0001679	Paxs	599.55	Joback Method
dvisc	0.0002940	Paxs	539.47	Joback Method
dvisc	0.0005924	Paxs	479.38	Joback Method

Sources

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=U381208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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