

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

Inchi:	InChI=1S/C19H28O5/c1-4-8-17(15(2)3)24-19(21)12-11-18(20)23-14-13-22-16-9-6-5-7-10
InchiKey:	OGRHOWGHCGBQEM-UHFFFAOYSA-N
Formula:	C19H28O5
SMILES:	CCCC(OC(=O)CCC(=O)OCCOc1ccccc1)C(C)C
Mol. weight [g/mol]:	336.42

Physical Properties

Property code	Value	Unit	Source
gf	-356.21	kJ/mol	Joback Method
hf	-831.34	kJ/mol	Joback Method
hfus	38.72	kJ/mol	Joback Method
hvap	80.11	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.757		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinsol	2320.00		NIST Webbook
tb	834.92	K	Joback Method
tc	1038.21	K	Joback Method
tf	466.86	K	Joback Method
vc	1.046	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.94	J/molxK	834.92	Joback Method
cpg	865.75	J/molxK	868.80	Joback Method
cpg	880.35	J/molxK	902.68	Joback Method
cpg	893.74	J/molxK	936.56	Joback Method
cpg	905.95	J/molxK	970.44	Joback Method
cpg	916.99	J/molxK	1004.32	Joback Method
cpg	926.87	J/molxK	1038.21	Joback Method
dvisc	0.0007125	Paxs	466.86	Joback Method
dvisc	0.0003322	Paxs	528.20	Joback Method

dvisc	0.0001815	Paxs	589.55	Joback Method
dvisc	0.0001112	Paxs	650.89	Joback Method
dvisc	0.0000741	Paxs	712.23	Joback Method
dvisc	0.0000527	Paxs	773.58	Joback Method
dvisc	0.0000394	Paxs	834.92	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=U381196&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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