Succinic acid, hept-2-yl 2-methoxy-5-methylphenyl ester

Inchi: InChI=1S/C19H28O5/c1-5-6-7-8-15(3)23-18(20)11-12-19(21)24-17-13-14(2)9-10-16(17)2

InchiKey: UOYBWQDIOPIYRO-UHFFFAOYSA-N

Formula: C19H28O5

SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-373.03	kJ/mol	Joback Method
hf	-849.00	kJ/mol	Joback Method
hfus	41.47	kJ/mol	Joback Method
hvap	81.82	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.201		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook
tb	845.32	K	Joback Method
tc	1048.37	K	Joback Method
tf	506.90	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.95	J/mol×K	845.32	Joback Method
cpg	863.44	J/mol×K	879.16	Joback Method
cpg	877.73	J/mol×K	913.00	Joback Method
cpg	890.84	J/mol×K	946.84	Joback Method
cpg	902.75	J/mol×K	980.68	Joback Method
cpg	913.49	J/mol×K	1014.53	Joback Method
cpg	923.04	J/mol×K	1048.37	Joback Method
dvisc	0.0004436	Pa×s	506.90	Joback Method

dvisc	0.0002488	Pa×s	563.30	Joback Method
dvisc	0.0001551	Pa×s	619.71	Joback Method
dvisc	0.0001046	Pa×s	676.11	Joback Method
dvisc	0.0000749	Pa×s	732.51	Joback Method
dvisc	0.0000563	Pa×s	788.92	Joback Method
dvisc	0.0000440	Pa×s	845.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390959&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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