Succinic acid, phenyl 2-methylbutyl ester

Inchi: InChI=1S/C15H20O4/c1-3-12(2)11-18-14(16)9-10-15(17)19-13-7-5-4-6-8-13/h4-8,12H,3,
InchiKey: SRADRAUVJACILN-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCC(C)COC(=O)CCC(=O)Oc1ccccc1
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	-282.45	kJ/mol	Joback Method
hf	-611.28	kJ/mol	Joback Method
hfus	30.70	kJ/mol	Joback Method
hvap	69.18	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.961		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1968.00		NIST Webbook
tb	721.42	K	Joback Method
tc	927.47	K	Joback Method
tf	414.55	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.99	J/mol×K	721.42	Joback Method
cpg	610.15	J/mol×K	755.76	Joback Method
cpg	624.31	J/mol×K	790.10	Joback Method
cpg	637.50	J/mol×K	824.44	Joback Method
cpg	649.73	J/mol×K	858.78	Joback Method
cpg	661.01	J/mol×K	893.13	Joback Method
cpg	671.36	J/mol×K	927.47	Joback Method
dvisc	0.0013106	Pa×s	414.55	Joback Method
dvisc	0.0006703	Pa×s	465.69	Joback Method

dvisc	0.0003915	Pa×s	516.84	Joback Method
dvisc	0.0002519	Pa×s	567.99	Joback Method
dvisc	0.0001744	Pa×s	619.13	Joback Method
dvisc	0.0001276	Pa×s	670.27	Joback Method
dvisc	0.0000977	Pa×s	721.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357988&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

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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