Succinic acid, 3-methylbut-2-yl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C17H24O4/c1-11(2)14(5)20-16(18)9-10-17(19)21-15-8-6-7-12(3)13(15)4/h6-8,

InchiKey: ZKDMGKMCPHTIES-UHFFFAOYSA-N

Formula: C17H24O4

SMILES: Cc1cccc(OC(=O)CCC(=O)OC(C)C(C)C)c1C

Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-287.31	kJ/mol	Joback Method
hf	-680.78	kJ/mol	Joback Method
hfus	31.58	kJ/mol	Joback Method
hvap	74.57	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.577		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook
tb	776.70	K	Joback Method
tc	983.40	K	Joback Method
tf	447.13	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.68	J/mol×K	776.70	Joback Method
cpg	720.42	J/mol×K	811.15	Joback Method
cpg	735.09	J/mol×K	845.60	Joback Method
cpg	748.69	J/mol×K	880.05	Joback Method
cpg	761.24	J/mol×K	914.50	Joback Method
cpg	772.74	J/mol×K	948.95	Joback Method
cpg	783.21	J/mol×K	983.40	Joback Method
dvisc	0.0008685	Pa×s	447.13	Joback Method

dvisc	0.0004536	Pa×s	502.06	Joback Method
dvisc	0.0002693	Pa×s	556.99	Joback Method
dvisc	0.0001756	Pa×s	611.91	Joback Method
dvisc	0.0001228	Pa×s	666.84	Joback Method
dvisc	0.0000907	Pa×s	721.77	Joback Method
dvisc	0.0000700	Pa×s	776.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390016&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