

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:	<chem>Cc1cccc(OC(=O)CCC(=O)OC(C)C(C)C)c1C</chem>
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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004536	Paxs	502.06	Joback Method
dvisc	0.0002693	Paxs	556.99	Joback Method
dvisc	0.0001756	Paxs	611.91	Joback Method
dvisc	0.0001228	Paxs	666.84	Joback Method
dvisc	0.0000907	Paxs	721.77	Joback Method
dvisc	0.0000700	Paxs	776.70	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=U390016&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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