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

Inchi: InChI=1S/C16H22O5/c1-11(2)12(3)20-15(17)8-9-16(18)21-14-7-5-6-13(10-14)19-4/h5-7,

InchiKey: ZJRRGYJXVQOEAR-UHFFFAOYSA-N

Formula: C16H22O5

SMILES: COc1cccc(OC(=O)CCC(=O)OC(C)C(C)C)c1

Mol. weight [g/mol]: 294.34

Physical Properties

Property code	Value	Unit	Source
gf	-391.10	kJ/mol	Joback Method
hf	-780.89	kJ/mol	Joback Method
hfus	30.56	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.968		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	771.26	K	Joback Method
tc	977.91	K	Joback Method
tf	445.57	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.40	J/mol×K	771.26	Joback Method
cpg	692.56	J/mol×K	805.70	Joback Method
cpg	706.64	J/mol×K	840.14	Joback Method
cpg	719.65	J/mol×K	874.58	Joback Method
cpg	731.56	J/mol×K	909.03	Joback Method
cpg	742.40	J/mol×K	943.47	Joback Method
cpg	752.15	J/mol×K	977.91	Joback Method
dvisc	0.0008051	Pa×s	445.57	Joback Method

dvisc	0.0004136	Pa×s	499.85	Joback Method
dvisc	0.0002420	Pa×s	554.13	Joback Method
dvisc	0.0001559	Pa×s	608.41	Joback Method
dvisc	0.0001079	Pa×s	662.70	Joback Method
dvisc	0.0000789	Pa×s	716.98	Joback Method
dvisc	0.0000604	Pa×s	771.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390976&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