Succinic acid, 3-methoxybenzyl octyl ester

Inchi: InChI=1S/C20H30O5/c1-3-4-5-6-7-8-14-24-19(21)12-13-20(22)25-16-17-10-9-11-18(15-1
InchiKey: DQVZBFAZBFBLPE-UHFFFAOYSA-N
Formula: C20H30O5
SMILES: CCCCCCCCOC(=O)CCC(=O)OCc1cccc(OC)c1
Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-352.54	kJ/mol	Joback Method
hf	-852.89	kJ/mol	Joback Method
hfus	47.97	kJ/mol	Joback Method
hvap	83.77	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.422		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	863.66	K	Joback Method
tc	1065.19	K	Joback Method
tf	520.65	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.10	J/mol×K	863.66	Joback Method
cpg	922.75	J/mol×K	897.25	Joback Method
cpg	937.18	J/mol×K	930.84	Joback Method
cpg	950.41	J/mol×K	964.43	Joback Method
cpg	962.45	J/mol×K	998.02	Joback Method
cpg	973.30	J/mol×K	1031.61	Joback Method
cpg	982.99	J/mol×K	1065.19	Joback Method
dvisc	0.0004161	Pa×s	520.65	Joback Method

dvisc	0.0002338	Pa×s	577.82	Joback Method
dvisc	0.0001457	Pa×s	634.99	Joback Method
dvisc	0.0000982	Pa×s	692.15	Joback Method
dvisc	0.0000703	Pa×s	749.32	Joback Method
dvisc	0.0000527	Pa×s	806.49	Joback Method
dvisc	0.0000411	Pa×s	863.66	Joback Method

Sources

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=U381258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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