Succinic acid, 2-methylbenzyl undecyl ester

Inchi: InChI=1S/C23H36O4/c1-3-4-5-6-7-8-9-10-13-18-26-22(24)16-17-23(25)27-19-21-15-12-1
InchiKey: OILGQTZXDLOBGD-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCCCCCCCOC(=O)CCC(=O)OCc1ccccc1C
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-222.28	kJ/mol	Joback Method
hf	-782.59	kJ/mol	Joback Method
hfus	54.55	kJ/mol	Joback Method
hvap	88.04	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.892		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	909.88	K	Joback Method
tc	1115.88	K	Joback Method
tf	532.23	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.08	J/mol×K	909.88	Joback Method
cpg	1129.40	J/mol×K	1081.55	Joback Method
cpg	1117.59	J/mol×K	1047.21	Joback Method
cpg	1104.59	J/mol×K	1012.88	Joback Method
cpg	1090.35	J/mol×K	978.55	Joback Method
cpg	1074.86	J/mol×K	944.21	Joback Method
cpg	1140.05	J/mol×K	1115.88	Joback Method
dvisc	0.0000357	Pa×s	909.88	Joback Method

dvisc	0.0000463	Pa×s	846.94	Joback Method
dvisc	0.0000627	Pa×s	784.00	Joback Method
dvisc	0.0000895	Pa×s	721.06	Joback Method
dvisc	0.0001367	Pa×s	658.11	Joback Method
dvisc	0.0002285	Pa×s	595.17	Joback Method
dvisc	0.0004311	Pa×s	532.23	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U381032&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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