Succinic acid, hexadecyl 2-methylbenzyl ester

Inchi: InChI=1S/C28H46O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-23-31-27(29)21-22-28(30)3
InchiKey: SIRMDADPZKAREQ-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccccc1C
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-180.18	kJ/mol	Joback Method
hf	-885.79	kJ/mol	Joback Method
hfus	67.50	kJ/mol	Joback Method
hvap	99.17	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.843		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	817.26	kPa	Joback Method
rinpol	3237.00		NIST Webbook
rinpol	3237.00		NIST Webbook
tb	1024.28	K	Joback Method
tc	1259.00	K	Joback Method
tf	588.58	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.60	J/mol×K	1024.28	Joback Method
cpg	1387.84	J/mol×K	1063.40	Joback Method
cpg	1404.30	J/mol×K	1102.52	Joback Method
cpg	1419.05	J/mol×K	1141.64	Joback Method
cpg	1432.16	J/mol×K	1180.76	Joback Method
cpg	1443.70	J/mol×K	1219.88	Joback Method
cpg	1453.73	J/mol×K	1259.00	Joback Method
dvisc	0.0002368	Pa×s	588.58	Joback Method

dvisc	0.0001195	Pa×s	661.20	Joback Method
dvisc	0.0000690	Pa×s	733.81	Joback Method
dvisc	0.0000440	Pa×s	806.43	Joback Method
dvisc	0.0000302	Pa×s	879.05	Joback Method
dvisc	0.0000220	Pa×s	951.66	Joback Method
dvisc	0.0000167	Pa×s	1024.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U381037&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