Succinic acid, hexadecyl 5-methylhex-2-yl ester

Inchi: InChI=1S/C27H52O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-30-26(28)21-22-27(2

InchiKey: PHBKMKHXZNMWPE-UHFFFAOYSA-N

Formula: C27H52O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OC(C)CCC(C)C

Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-296.26	kJ/mol	Joback Method
hf	-1100.77	kJ/mol	Joback Method
hfus	64.21	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	8.159		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	729.67	kPa	Joback Method
rinpol	2909.00		NIST Webbook
rinpol	2909.00		NIST Webbook
tb	968.86	K	Joback Method
tc	1194.47	K	Joback Method
tf	508.37	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.37	J/mol×K	968.86	Joback Method
cpg	1431.98	J/mol×K	1006.46	Joback Method
cpg	1451.77	J/mol×K	1044.06	Joback Method
cpg	1469.79	J/mol×K	1081.67	Joback Method
cpg	1486.11	J/mol×K	1119.27	Joback Method
cpg	1500.78	J/mol×K	1156.87	Joback Method
cpg	1513.86	J/mol×K	1194.47	Joback Method
dvisc	0.0004716	Pa×s	508.37	Joback Method

dvisc	0.0001832	Pa×s	585.12	Joback Method
dvisc	0.0000886	Pa×s	661.87	Joback Method
dvisc	0.0000498	Pa×s	738.62	Joback Method
dvisc	0.0000312	Pa×s	815.36	Joback Method
dvisc	0.0000212	Pa×s	892.11	Joback Method
dvisc	0.0000153	Pa×s	968.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382383&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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