Succinic acid, dec-4-enyl nonyl ester

Inchi: InChI=1S/C23H42O4/c1-3-5-7-9-11-13-15-17-21-27-23(25)19-18-22(24)26-20-16-14-12-
InchiKey: XKDDNNDEPTVVIJ-ACCUITESSA-N
Formula: C23H42O4
SMILES: CCCCCC=CCCCOC(=O)CCC(=O)OCCCCCCCCC
Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-244.84	kJ/mol	Joback Method
hf	-890.43	kJ/mol	Joback Method
hfus	61.10	kJ/mol	Joback Method
hvap	85.06	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.520		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	928.37	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	882.38	K	Joback Method
tc	1080.29	K	Joback Method
tf	488.21	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1127.87	J/mol×K	882.38	Joback Method
cpg	1146.91	J/mol×K	915.36	Joback Method
cpg	1164.75	J/mol×K	948.35	Joback Method
cpg	1181.44	J/mol×K	981.33	Joback Method
cpg	1197.00	J/mol×K	1014.32	Joback Method
cpg	1211.47	J/mol×K	1047.30	Joback Method
cpg	1224.91	J/mol×K	1080.29	Joback Method
dvisc	0.0005530	Pa×s	488.21	Joback Method

dvisc	0.0002548	Pa×s	553.90	Joback Method
dvisc	0.0001384	Pa×s	619.60	Joback Method
dvisc	0.0000845	Pa×s	685.30	Joback Method
dvisc	0.0000562	Pa×s	750.99	Joback Method
dvisc	0.0000400	Pa×s	816.68	Joback Method
dvisc	0.0000299	Pa×s	882.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353469&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

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