Succinic acid, docosyl pentyl ester

Inchi: InChI=1S/C31H60O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-29-3
InchiKey: GTUZIDUONDAKOQ-UHFFFAOYSA-N
Formula: C31H60O4
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCCCCC
Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	-257.70	kJ/mol	Joback Method
hf	-1172.77	kJ/mol	Joback Method
hfus	81.62	kJ/mol	Joback Method
hvap	102.91	kJ/mol	Joback Method
log10ws	-10.52		Crippen Method
logp	9.865		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	594.30	kPa	Joback Method
rinpol	3443.00		NIST Webbook
rinpol	3443.00		NIST Webbook
tb	1061.26	K	Joback Method
tc	1344.42	K	Joback Method
tf	583.45	K	Joback Method
vc	1.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.89	J/mol×K	1061.26	Joback Method
cpg	1696.10	J/mol×K	1108.45	Joback Method
cpg	1718.46	J/mol×K	1155.65	Joback Method
cpg	1738.13	J/mol×K	1202.84	Joback Method
cpg	1755.25	J/mol×K	1250.03	Joback Method
cpg	1769.95	J/mol×K	1297.22	Joback Method
cpg	1782.40	J/mol×K	1344.42	Joback Method
dvisc	0.0002077	Pa×s	583.45	Joback Method

dvisc	0.0000918	Pa×s	663.08	Joback Method
dvisc	0.0000484	Pa×s	742.72	Joback Method
dvisc	0.0000288	Pa×s	822.36	Joback Method
dvisc	0.0000188	Pa×s	901.99	Joback Method
dvisc	0.0000132	Pa×s	981.62	Joback Method
dvisc	0.0000097	Pa×s	1061.26	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=U349575&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