9-Octadecenylsuccinic acid

Other names: Octadecenylsuccinic acid
dihydro-3-(octadecenyl)furan-2,5-dione
Inchi: InChI=1S/C22H40O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20(22(25)26)19-21
InchiKey: XACKAZKMZQZZDT-MDZDMXLPSA-N
Formula: C22H40O4
SMILES: CCCCCCCCC=CCCCCCCCCC(CC(=O)O)C(=O)O
Mol. weight [g/mol]: 368.55
CAS: 28777-98-2

Physical Properties

Property code	Value	Unit	Source
gf	-319.34	kJ/mol	Joback Method
hf	-915.09	kJ/mol	Joback Method
hfus	60.79	kJ/mol	Joback Method
hvap	110.99	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.590		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
tb	998.58	K	Joback Method
tc	1237.82	K	Joback Method
tf	539.12	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.01	J/mol×K	998.58	Joback Method
cpg	1156.88	J/mol×K	1038.45	Joback Method
cpg	1173.62	J/mol×K	1078.33	Joback Method
cpg	1189.37	J/mol×K	1118.20	Joback Method
cpg	1204.22	J/mol×K	1158.07	Joback Method
cpg	1218.29	J/mol×K	1197.94	Joback Method
cpg	1231.70	J/mol×K	1237.82	Joback Method

dvisc	0.0001898	Pa×s	539.12	Joback Method
dvisc	0.0000441	Pa×s	615.70	Joback Method
dvisc	0.0000141	Pa×s	692.27	Joback Method
dvisc	0.0000057	Pa×s	768.85	Joback Method
dvisc	0.0000027	Pa×s	845.43	Joback Method
dvisc	0.0000015	Pa×s	922.00	Joback Method
dvisc	0.0000009	Pa×s	998.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28777982&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume