Sebacic acid, 10-chlorodecyl octyl ester

Inchi: InChI=1S/C28H53ClO4/c1-2-3-4-5-15-20-25-32-27(30)22-17-12-8-9-13-18-23-28(31)33-2
InchiKey: CDEDJKAMRYIXKT-UHFFFAOYSA-N
Formula: C28H53ClO4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCl
Mol. weight [g/mol]: 489.17

Physical Properties

Property code	Value	Unit	Source
gf	-294.89	kJ/mol	Joback Method
hf	-1126.59	kJ/mol	Joback Method
hfus	78.05	kJ/mol	Joback Method
hvap	100.62	kJ/mol	Joback Method
log10ws	-9.42		Crippen Method
logp	8.914		Crippen Method
mcvol	432.500	ml/mol	McGowan Method
pc	674.30	kPa	Joback Method
rinpol	3528.00		NIST Webbook
rinpol	3528.00		NIST Webbook
tb	1030.05	K	Joback Method
tc	1285.34	K	Joback Method
tf	579.56	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1503.95	J/mol×K	1030.05	Joback Method
cpg	1525.75	J/mol×K	1072.60	Joback Method
cpg	1545.36	J/mol×K	1115.15	Joback Method
cpg	1562.86	J/mol×K	1157.70	Joback Method
cpg	1578.35	J/mol×K	1200.25	Joback Method
cpg	1591.94	J/mol×K	1242.80	Joback Method
cpg	1603.70	J/mol×K	1285.34	Joback Method
dvisc	0.0002392	Pa×s	579.56	Joback Method

dvisc	0.0001116	Pa×s	654.64	Joback Method
dvisc	0.0000609	Pa×s	729.72	Joback Method
dvisc	0.0000372	Pa×s	804.81	Joback Method
dvisc	0.0000247	Pa×s	879.89	Joback Method
dvisc	0.0000175	Pa×s	954.97	Joback Method
dvisc	0.0000130	Pa×s	1030.05	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=U355344&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