Adipic acid, 2-chloropropyl octadecyl ester

Inchi: InChI=1S/C27H51ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-31-26(29)21-18
InchiKey: NFQPHOFHQFHPTI-UHFFFAOYSA-N
Formula: C27H51ClO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 475.14

Physical Properties

Property code	Value	Unit	Source
gf	-305.75	kJ/mol	Joback Method
hf	-1111.23	kJ/mol	Joback Method
hfus	71.93	kJ/mol	Joback Method
hvap	98.01	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	8.522		Crippen Method
mcvol	418.410	ml/mol	McGowan Method
pc	712.25	kPa	Joback Method
rinpol	3240.00		NIST Webbook
rinpol	3240.00		NIST Webbook
tb	1006.73	K	Joback Method
tc	1247.18	K	Joback Method
tf	553.29	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1439.83	J/mol×K	1006.73	Joback Method
cpg	1525.16	J/mol×K	1207.11	Joback Method
cpg	1511.72	J/mol×K	1167.03	Joback Method
cpg	1496.54	J/mol×K	1126.96	Joback Method
cpg	1479.54	J/mol×K	1086.88	Joback Method
cpg	1460.66	J/mol×K	1046.81	Joback Method
cpg	1536.95	J/mol×K	1247.18	Joback Method
dvisc	0.0000139	Pa×s	1006.73	Joback Method

dvisc	0.0000189	Pa×s	931.16	Joback Method
dvisc	0.0000272	Pa×s	855.58	Joback Method
dvisc	0.0000418	Pa×s	780.01	Joback Method
dvisc	0.0000704	Pa×s	704.44	Joback Method
dvisc	0.0001346	Pa×s	628.86	Joback Method
dvisc	0.0003072	Pa×s	553.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353553&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume