Adipic acid, 8-chloroctyl tridecyl ester

Inchi: InChI=1S/C27H51ClO4/c1-2-3-4-5-6-7-8-9-11-14-19-24-31-26(29)21-16-17-22-27(30)32-
InchiKey: KWSLVIWMUBDKCJ-UHFFFAOYSA-N
Formula: C27H51ClO4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 475.14

Physical Properties

Property code	Value	Unit	Source
gf	-303.31	kJ/mol	Joback Method
hf	-1105.95	kJ/mol	Joback Method
hfus	75.46	kJ/mol	Joback Method
hvap	98.39	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	8.524		Crippen Method
mcvol	418.410	ml/mol	McGowan Method
pc	709.22	kPa	Joback Method
rinpol	3362.00		NIST Webbook
rinpol	3362.00		NIST Webbook
tb	1007.17	K	Joback Method
tc	1250.03	K	Joback Method
tf	568.29	K	Joback Method
vc	1.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1439.54	J/mol×K	1007.17	Joback Method
cpg	1526.02	J/mol×K	1209.55	Joback Method
cpg	1512.38	J/mol×K	1169.08	Joback Method
cpg	1496.99	J/mol×K	1128.60	Joback Method
cpg	1479.77	J/mol×K	1088.12	Joback Method
cpg	1460.65	J/mol×K	1047.65	Joback Method
cpg	1537.98	J/mol×K	1250.03	Joback Method
dvisc	0.0000153	Pa×s	1007.17	Joback Method

dvisc	0.0000205	Pa×s	934.02	Joback Method
dvisc	0.0000289	Pa×s	860.88	Joback Method
dvisc	0.0000434	Pa×s	787.73	Joback Method
dvisc	0.0000707	Pa×s	714.58	Joback Method
dvisc	0.0001289	Pa×s	641.44	Joback Method
dvisc	0.0002741	Pa×s	568.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349768&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