Adipic acid, 8-chloroctyl dodecyl ester

Inchi: InChI=1S/C26H49ClO4/c1-2-3-4-5-6-7-8-10-13-18-23-30-25(28)20-15-16-21-26(29)31-24
InchiKey: WZKJRQQTUGHAKP-UHFFFAOYSA-N
Formula: C26H49ClO4
SMILES: CCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 461.12

Physical Properties

Property code	Value	Unit	Source
gf	-311.73	kJ/mol	Joback Method
hf	-1085.31	kJ/mol	Joback Method
hfus	72.87	kJ/mol	Joback Method
hvap	96.17	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	8.134		Crippen Method
mcvol	404.320	ml/mol	McGowan Method
pc	746.92	kPa	Joback Method
rinpol	3268.00		NIST Webbook
rinpol	3268.00		NIST Webbook
tb	984.29	K	Joback Method
tc	1216.16	K	Joback Method
tf	557.02	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1375.47	J/mol×K	984.29	Joback Method
cpg	1395.92	J/mol×K	1022.94	Joback Method
cpg	1414.58	J/mol×K	1061.58	Joback Method
cpg	1431.50	J/mol×K	1100.23	Joback Method
cpg	1446.76	J/mol×K	1138.87	Joback Method
cpg	1460.41	J/mol×K	1177.52	Joback Method
cpg	1472.51	J/mol×K	1216.16	Joback Method
dvisc	0.0003134	Pa×s	557.02	Joback Method

dvisc	0.0001486	Pa×s	628.23	Joback Method
dvisc	0.0000820	Pa×s	699.44	Joback Method
dvisc	0.0000505	Pa×s	770.65	Joback Method
dvisc	0.0000338	Pa×s	841.87	Joback Method
dvisc	0.0000241	Pa×s	913.08	Joback Method
dvisc	0.0000180	Pa×s	984.29	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=U349767&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