Adipic acid, 2-chloropropyl pentadecyl ester

Inchi: InChI=1S/C24H45ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-20-28-23(26)18-15-16-19-24
InchiKey: SNFWTKACFXBQLM-UHFFFAOYSA-N
Formula: C24H45ClO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 433.06

Physical Properties

Property code	Value	Unit	Source
gf	-331.01	kJ/mol	Joback Method
hf	-1049.31	kJ/mol	Joback Method
hfus	64.16	kJ/mol	Joback Method
hvap	91.33	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	7.352		Crippen Method
mcvol	376.140	ml/mol	McGowan Method
pc	835.79	kPa	Joback Method
rinpol	2930.00		NIST Webbook
rinpol	2930.00		NIST Webbook
tb	938.09	K	Joback Method
tc	1150.89	K	Joback Method
tf	519.48	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.90	J/mol×K	938.09	Joback Method
cpg	1268.05	J/mol×K	973.56	Joback Method
cpg	1285.71	J/mol×K	1009.02	Joback Method
cpg	1301.93	J/mol×K	1044.49	Joback Method
cpg	1316.73	J/mol×K	1079.96	Joback Method
cpg	1330.17	J/mol×K	1115.42	Joback Method
cpg	1342.28	J/mol×K	1150.89	Joback Method
dvisc	0.0004616	Pa×s	519.48	Joback Method

dvisc	0.0002071	Pa×s	589.25	Joback Method
dvisc	0.0001101	Pa×s	659.02	Joback Method
dvisc	0.0000661	Pa×s	728.79	Joback Method
dvisc	0.0000434	Pa×s	798.55	Joback Method
dvisc	0.0000304	Pa×s	868.32	Joback Method
dvisc	0.0000225	Pa×s	938.09	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=U353551&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