

Adipic acid, 2-chloropropyl tetradecyl ester

Inchi: InChI=1S/C23H43ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-16-19-27-22(25)17-14-15-18-23(20)
InchiKey: YONSGQZDUNQEJY-UHFFFAOYSA-N
Formula: C23H43ClO4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 419.04

Physical Properties

Property code	Value	Unit	Source
gf	-339.43	kJ/mol	Joback Method
hf	-1028.67	kJ/mol	Joback Method
hfus	61.57	kJ/mol	Joback Method
hvap	89.10	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.962		Crippen Method
mcvol	362.050	ml/mol	McGowan Method
pc	884.19	kPa	Joback Method
rinsol	2826.00		NIST Webbook
tb	915.21	K	Joback Method
tc	1121.16	K	Joback Method
tf	508.21	K	Joback Method
vc	1.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.14	J/molxK	915.21	Joback Method
cpg	1204.81	J/molxK	949.54	Joback Method
cpg	1222.10	J/molxK	983.86	Joback Method
cpg	1238.06	J/molxK	1018.19	Joback Method
cpg	1252.71	J/molxK	1052.51	Joback Method
cpg	1266.08	J/molxK	1086.84	Joback Method
cpg	1278.23	J/molxK	1121.16	Joback Method
dvisc	0.0005261	Paxs	508.21	Joback Method
dvisc	0.0002381	Paxs	576.04	Joback Method

dvisc	0.0001273	Paxs	643.88	Joback Method
dvisc	0.0000767	Paxs	711.71	Joback Method
dvisc	0.0000505	Paxs	779.54	Joback Method
dvisc	0.0000355	Paxs	847.38	Joback Method
dvisc	0.0000263	Paxs	915.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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