Adipic acid, di(2-chloropropyl) ester

Inchi: InChI=1S/C12H20Cl2O4/c1-9(13)7-17-11(15)5-3-4-6-12(16)18-8-10(2)14/h9-10H,3-8H2,
InchiKey: DINLBXUNHXSUJJ-UHFFFAOYSA-N
Formula: C12H20Cl2O4
SMILES: CC(Cl)COC(=O)CCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 299.19

Physical Properties

Property code	Value	Unit	Source
gf	-446.42	kJ/mol	Joback Method
hf	-822.65	kJ/mol	Joback Method
hfus	33.76	kJ/mol	Joback Method
hvap	68.61	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.888		Crippen Method
mcvol	219.300	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1987.00		NIST Webbook
tb	700.52	K	Joback Method
tc	892.04	K	Joback Method
tf	399.16	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.07	J/mol×K	700.52	Joback Method
cpg	587.54	J/mol×K	732.44	Joback Method
cpg	600.25	J/mol×K	764.36	Joback Method
cpg	612.20	J/mol×K	796.28	Joback Method
cpg	623.41	J/mol×K	828.20	Joback Method
cpg	633.88	J/mol×K	860.12	Joback Method
cpg	643.60	J/mol×K	892.04	Joback Method
dvisc	0.0017341	Pa×s	399.16	Joback Method
dvisc	0.0008385	Pa×s	449.39	Joback Method

dvisc	0.0004692	Pa×s	499.61	Joback Method
dvisc	0.0002919	Pa×s	549.84	Joback Method
dvisc	0.0001967	Pa×s	600.07	Joback Method
dvisc	0.0001408	Pa×s	650.29	Joback Method
dvisc	0.0001058	Pa×s	700.52	Joback Method

Sources

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=U353554&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/16-415-3/Adipic-acid-di-2-chloropropyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:52:22.833718916 +0000 UTC m=+3286005.470688165.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.