Adipic acid, 2,2-dichloroethyl pentyl ester

Inchi: InChI=1S/C13H22Cl2O4/c1-2-3-6-9-18-12(16)7-4-5-8-13(17)19-10-11(14)15/h11H,2-10H
InchiKey: YRKPIUINHGBECT-UHFFFAOYSA-N
Formula: C13H22Cl2O4
SMILES: CCCCCOC(=O)CCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 313.22

Physical Properties

Property code	Value	Unit	Source
gf	-435.56	kJ/mol	Joback Method
hf	-838.01	kJ/mol	Joback Method
hfus	39.87	kJ/mol	Joback Method
hvap	71.23	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.627		Crippen Method
mcvol	233.390	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	1994.00		NIST Webbook
rinpol	1994.00		NIST Webbook
tb	723.84	K	Joback Method
tc	911.74	K	Joback Method
tf	425.43	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.11	J/mol×K	723.84	Joback Method
cpg	688.12	J/mol×K	880.42	Joback Method
cpg	677.44	J/mol×K	849.10	Joback Method
cpg	666.00	J/mol×K	817.79	Joback Method
cpg	653.80	J/mol×K	786.47	Joback Method
cpg	640.84	J/mol×K	755.16	Joback Method
cpg	698.07	J/mol×K	911.74	Joback Method
dvisc	0.0000995	Pa×s	723.84	Joback Method

dvisc	0.0001304	Pa×s	674.10	Joback Method
dvisc	0.0001784	Pa×s	624.37	Joback Method
dvisc	0.0002577	Pa×s	574.63	Joback Method
dvisc	0.0003990	Pa×s	524.90	Joback Method
dvisc	0.0006770	Pa×s	475.16	Joback Method
dvisc	0.0012999	Pa×s	425.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353579&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

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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