Adipic acid, 2,2-dichloroethyl dodecyl ester

Inchi: InChI=1S/C20H36Cl2O4/c1-2-3-4-5-6-7-8-9-10-13-16-25-19(23)14-11-12-15-20(24)26-17
InchiKey: LGDOJQYVUWBOOP-UHFFFAOYSA-N
Formula: C20H36Cl2O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 411.40

Physical Properties

Property code	Value	Unit	Source
gf	-376.62	kJ/mol	Joback Method
hf	-982.49	kJ/mol	Joback Method
hfus	58.00	kJ/mol	Joback Method
hvap	86.81	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	6.358		Crippen Method
mcvol	332.020	ml/mol	McGowan Method
pc	1032.57	kPa	Joback Method
rinpol	2695.00		NIST Webbook
tb	884.00	K	Joback Method
tc	1082.74	K	Joback Method
tf	504.32	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.76	J/mol×K	884.00	Joback Method
cpg	1101.56	J/mol×K	1049.62	Joback Method
cpg	1089.62	J/mol×K	1016.50	Joback Method
cpg	1076.59	J/mol×K	983.37	Joback Method
cpg	1062.45	J/mol×K	950.25	Joback Method
cpg	1047.19	J/mol×K	917.12	Joback Method
cpg	1112.45	J/mol×K	1082.74	Joback Method
dvisc	0.0000352	Pa×s	884.00	Joback Method
dvisc	0.0000470	Pa×s	820.72	Joback Method

dvisc	0.0000659	Pa×s	757.44	Joback Method
dvisc	0.0000981	Pa×s	694.16	Joback Method
dvisc	0.0001583	Pa×s	630.88	Joback Method
dvisc	0.0002842	Pa×s	567.60	Joback Method
dvisc	0.0005909	Pa×s	504.32	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353586&Units=SI

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