Adipic acid, 8-chloroctyl isohexyl ester

Inchi: InChI=1S/C20H37ClO4/c1-18(2)12-11-17-25-20(23)14-8-7-13-19(22)24-16-10-6-4-3-5-9-
InchiKey: FMZUTOFLYCLHDY-UHFFFAOYSA-N
Formula: C20H37ClO4
SMILES: CC(C)CCCOC(=O)CCCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 376.96

Physical Properties

Property code	Value	Unit	Source
gf	-364.69	kJ/mol	Joback Method
hf	-966.75	kJ/mol	Joback Method
hfus	53.80	kJ/mol	Joback Method
hvap	82.42	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.649		Crippen Method
mcvol	319.780	ml/mol	McGowan Method
pc	1057.57	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
tb	846.57	K	Joback Method
tc	1037.93	K	Joback Method
tf	474.40	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.30	J/mol×K	846.57	Joback Method
cpg	1018.70	J/mol×K	878.46	Joback Method
cpg	1034.98	J/mol×K	910.36	Joback Method
cpg	1050.18	J/mol×K	942.25	Joback Method
cpg	1064.31	J/mol×K	974.15	Joback Method
cpg	1077.39	J/mol×K	1006.04	Joback Method
cpg	1089.45	J/mol×K	1037.93	Joback Method
dvisc	0.0007660	Pa×s	474.40	Joback Method

dvisc	0.0003564	Pa×s	536.43	Joback Method
dvisc	0.0001943	Pa×s	598.46	Joback Method
dvisc	0.0001187	Pa×s	660.48	Joback Method
dvisc	0.0000789	Pa×s	722.51	Joback Method
dvisc	0.0000560	Pa×s	784.54	Joback Method
dvisc	0.0000418	Pa×s	846.57	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=U349760&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