Adipic acid, 8-chloroctyl pentyl ester

Inchi: InChI=1S/C19H35ClO4/c1-2-3-11-16-23-18(21)13-8-9-14-19(22)24-17-12-7-5-4-6-10-15-
InchiKey: IIDRUMFLPGVZJE-UHFFFAOYSA-N
Formula: C19H35ClO4
SMILES: CCCCCOC(=O)CCCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 362.93

Physical Properties

Property code	Value	Unit	Source
gf	-370.67	kJ/mol	Joback Method
hf	-940.83	kJ/mol	Joback Method
hfus	54.74	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.403		Crippen Method
mcvol	305.690	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2553.00		NIST Webbook
rinpol	2553.00		NIST Webbook
tb	824.13	K	Joback Method
tc	1011.58	K	Joback Method
tf	478.13	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.55	J/mol×K	824.13	Joback Method
cpg	957.49	J/mol×K	855.37	Joback Method
cpg	973.41	J/mol×K	886.61	Joback Method
cpg	988.32	J/mol×K	917.85	Joback Method
cpg	1002.25	J/mol×K	949.09	Joback Method
cpg	1015.20	J/mol×K	980.33	Joback Method
cpg	1027.20	J/mol×K	1011.58	Joback Method
dvisc	0.0007414	Pa×s	478.13	Joback Method

dvisc	0.0003768	Pa×s	535.80	Joback Method
dvisc	0.0002184	Pa×s	593.46	Joback Method
dvisc	0.0001394	Pa×s	651.13	Joback Method
dvisc	0.0000957	Pa×s	708.80	Joback Method
dvisc	0.0000696	Pa×s	766.46	Joback Method
dvisc	0.0000529	Pa×s	824.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349759&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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