Adipic acid, 8-chloroctyl propyl ester

Inchi: InChI=1S/C17H31ClO4/c1-2-14-21-16(19)11-7-8-12-17(20)22-15-10-6-4-3-5-9-13-18/h2-
InchiKey: ININBCUUYLOIJC-UHFFFAOYSA-N
Formula: C17H31ClO4
SMILES: CCCOC(=O)CCCCC(=O)OCCCCCCCCCCl
Mol. weight [g/mol]: 334.88

Physical Properties

Property code	Value	Unit	Source
gf	-387.51	kJ/mol	Joback Method
hf	-899.55	kJ/mol	Joback Method
hfus	49.56	kJ/mol	Joback Method
hvap	76.13	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.623		Crippen Method
mcvol	277.510	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	778.37	K	Joback Method
tc	961.19	K	Joback Method
tf	455.59	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.48	J/mol×K	778.37	Joback Method
cpg	838.60	J/mol×K	808.84	Joback Method
cpg	853.83	J/mol×K	839.31	Joback Method
cpg	868.17	J/mol×K	869.78	Joback Method
cpg	881.62	J/mol×K	900.25	Joback Method
cpg	894.21	J/mol×K	930.72	Joback Method
cpg	905.95	J/mol×K	961.19	Joback Method
dvisc	0.0009196	Pa×s	455.59	Joback Method

dvisc	0.0004784	Pa×s	509.39	Joback Method
dvisc	0.0002820	Pa×s	563.18	Joback Method
dvisc	0.0001823	Pa×s	616.98	Joback Method
dvisc	0.0001263	Pa×s	670.78	Joback Method
dvisc	0.0000925	Pa×s	724.57	Joback Method
dvisc	0.0000707	Pa×s	778.37	Joback Method

Sources

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=U349756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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