Adipic acid, 8-chloroctyl heptyl ester

Inchi: InChI=1S/C21H39ClO4/c1-2-3-4-8-13-18-25-20(23)15-10-11-16-21(24)26-19-14-9-6-5-7-
InchiKey: MARYDTQHJDPBRX-UHFFFAOYSA-N
Formula: C21H39ClO4
SMILES: CCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 390.99

Physical Properties

Property code	Value	Unit	Source
gf	-353.83	kJ/mol	Joback Method
hf	-982.11	kJ/mol	Joback Method
hfus	59.92	kJ/mol	Joback Method
hvap	85.04	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.183		Crippen Method
mcvol	333.870	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook
tb	869.89	K	Joback Method
tc	1065.07	K	Joback Method
tf	500.67	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.81	J/mol×K	869.89	Joback Method
cpg	1079.61	J/mol×K	902.42	Joback Method
cpg	1096.23	J/mol×K	934.95	Joback Method
cpg	1111.70	J/mol×K	967.48	Joback Method
cpg	1126.05	J/mol×K	1000.01	Joback Method
cpg	1139.30	J/mol×K	1032.54	Joback Method
cpg	1151.48	J/mol×K	1065.07	Joback Method
dvisc	0.0005888	Pa×s	500.67	Joback Method

dvisc	0.0002928	Pa×s	562.21	Joback Method
dvisc	0.0001671	Pa×s	623.74	Joback Method
dvisc	0.0001055	Pa×s	685.28	Joback Method
dvisc	0.0000718	Pa×s	746.82	Joback Method
dvisc	0.0000519	Pa×s	808.35	Joback Method
dvisc	0.0000392	Pa×s	869.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349762&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