Adipic acid, 8-chloroctyl pentadecyl ester

Inchi: InChI=1S/C29H55ClO4/c1-2-3-4-5-6-7-8-9-10-11-13-16-21-26-33-28(31)23-18-19-24-29(
InchiKey: CXSPMWHMFPVBNF-UHFFFAOYSA-N
Formula: C29H55ClO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 503.20

Physical Properties

Property code	Value	Unit	Source
gf	-286.47	kJ/mol	Joback Method
hf	-1147.23	kJ/mol	Joback Method
hfus	80.64	kJ/mol	Joback Method
hvap	102.84	kJ/mol	Joback Method
log10ws	-9.84		Crippen Method
logp	9.304		Crippen Method
mcvol	446.590	ml/mol	McGowan Method
pc	641.90	kPa	Joback Method
rinpol	3572.00		NIST Webbook
tb	1052.93	K	Joback Method
tc	1322.23	K	Joback Method
tf	590.83	K	Joback Method
vc	1.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1568.65	J/mol×K	1052.93	Joback Method
cpg	1591.19	J/mol×K	1097.81	Joback Method
cpg	1611.29	J/mol×K	1142.70	Joback Method
cpg	1629.07	J/mol×K	1187.58	Joback Method
cpg	1644.63	J/mol×K	1232.46	Joback Method
cpg	1658.10	J/mol×K	1277.35	Joback Method
cpg	1669.60	J/mol×K	1322.23	Joback Method
dvisc	0.0002084	Pa×s	590.83	Joback Method
dvisc	0.0000964	Pa×s	667.85	Joback Method

dvisc	0.0000523	Pa×s	744.86	Joback Method
dvisc	0.0000318	Pa×s	821.88	Joback Method
dvisc	0.0000211	Pa×s	898.90	Joback Method
dvisc	0.0000149	Pa×s	975.91	Joback Method
dvisc	0.0000111	Pa×s	1052.93	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=U349770&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