

Adipic acid, 8-chlorooctyl heptadecyl ester

Inchi: InChI=1S/C31H59ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-23-28-35-30(33)25-20-21-
InchiKey: APFJXSZJOKTTKO-UHFFFAOYSA-N
Formula: C31H59ClO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]: 531.25

Physical Properties

Property code	Value	Unit	Source
gf	-269.63	kJ/mol	Joback Method
hf	-1188.51	kJ/mol	Joback Method
hfus	85.82	kJ/mol	Joback Method
hvap	107.30	kJ/mol	Joback Method
log10ws	-10.68		Crippen Method
logp	10.084		Crippen Method
mcvol	474.770	ml/mol	McGowan Method
pc	583.73	kPa	Joback Method
tb	1098.69	K	Joback Method
tc	1401.24	K	Joback Method
tf	613.37	K	Joback Method
vc	1.869	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1698.77	J/mol×K	1098.69	Joback Method
cpg	1722.93	J/mol×K	1149.12	Joback Method
cpg	1744.05	J/mol×K	1199.54	Joback Method
cpg	1762.29	J/mol×K	1249.97	Joback Method
cpg	1777.86	J/mol×K	1300.39	Joback Method
cpg	1790.93	J/mol×K	1350.82	Joback Method
cpg	1801.68	J/mol×K	1401.24	Joback Method
dvisc	0.0001571	Paxs	613.37	Joback Method
dvisc	0.0000716	Paxs	694.26	Joback Method
dvisc	0.0000384	Paxs	775.14	Joback Method

dvisc	0.0000232	Paxs	856.03	Joback Method
dvisc	0.0000153	Paxs	936.92	Joback Method
dvisc	0.0000108	Paxs	1017.80	Joback Method
dvisc	0.0000080	Paxs	1098.69	Joback Method

Sources

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=U349772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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